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Poly[hexa-μ-acetato-bis(dimethyl sulfoxide)trimanganese(II)]

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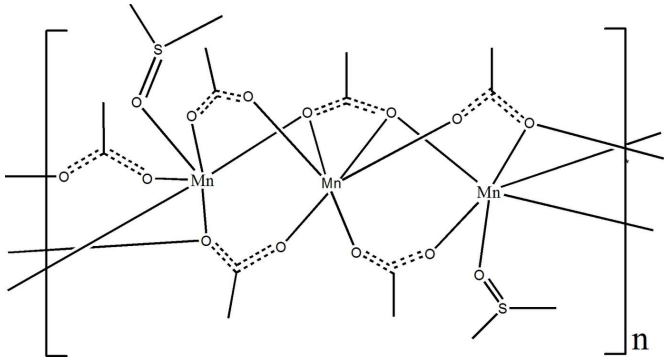
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.021; wR factor = 0.056; data-to-parameter ratio = 12.1.

In the title complex, $[Mn_3(CH_3CO_2)_6(C_2H_6SO)_2]_n$, the Mn^{II} ions exhibit similar MnO_6 octahedral coordination geometries but with different coordination environments. One type of Mn^{II} ion is surrounded by five acetate groups and a terminal dimethyl sulfoxide group, while the other lies on a twofold axis and is coordinated by six O atoms from three symmetry-related acetate ions. The acetate anions exhibit three independent bridging modes, which flexibly bridge the Mn^{II} ions along the c-axis direction, forming an infinite chain structure; the chains are further interconnected through weak C—H···O and C—H···S hydrogen-bonding interactions.

Related literature

For metal complexes of DMSO, see: Calligaris *et al.* (2004). For the structure of a related complex, see: Wang *et al.* (2000).



Experimental

Crystal data

$[Mn_3(C_2H_3O_2)_6(C_2H_6OS)_2]$
M_r = 675.34
Monoclinic, $C2$
a = 12.8475 (16) Å
b = 12.5439 (16) Å
c = 8.6095 (11) Å
β = 94.906 (2)°
V = 1382.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 293 K
0.41 × 0.36 × 0.29 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.883, T_{max} = 1.000
3821 measured reflections
1953 independent reflections
1919 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.056
S = 1.05
1953 reflections
161 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 653 Friedel pairs
Flack parameter: 0.034 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···O6^{i}	0.96	2.45	3.367 (4)	160
C2—H2B···S1^{ii}	0.96	2.99	3.841 (4)	147

Symmetry codes: (i) $x-\frac{1}{2}, y+\frac{1}{2}, z$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2332).

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supporting information

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Poly[hexa-μ-acetato-bis(dimethyl sulfoxide)trimanganese(II)]

Chong-Qing Wan, Nai-You Xiao and Zi-Jia Wang

S1. Comment

The coordination chemistry of dimethyl sulfoxid (DMSO) has been widely studied. Herein, we report the preparation and crystal strcuture of a new manganese(II) complex with dimethyl sulfoxide (DMSO). In the title complex, the two independent Mn^{II} ions (Mn1 and Mn2) exhibit a similar *O6*-octahedral coordination geometry with different coordination environments (Fig. 1). The Mn1 ion is surrounded by five acetates and one η^1-bonding DMSO, while the Mn2 lies on a two-fold axis and is coordinated by six oxygen atoms of three symmetry related acetate ions. The acetate anions exhibit three independent bridging modes, *syn*, *syn* η^1:η^1:μ^2-mode (C2-symmetric O3-containing acetate and O5-, O6-containing acetate), the *syn*, *syn*, *ant* η^1:η^2:μ^3-mode (O1-, O2-containing acetate) and the *syn*, *ant*, *syn*, *ant* η^2:η^2:μ^3-mode (C2-symmetric O7-containing acetate). The Mn1 and Mn2 ions are flexibly bridged by these anions and assemble into an infinite chain along the *c* direction (Fig. 2). The parallel arrays interconnect through C—H···O and C—H···S type H-bonding interactions (Table 1). In the termianl dimethyl sulfoxide, the S1═O4 of 1.501 (2)Å bond is slightly longer than that of the neat DMSO, which can be ascribed to the reduced bond order as that found in the protonated and η^1-coordinated alkyl sulfoxides (Calligaris *et al.*, 2004). The Mn1—O4 bond length of 2.153 (2)Å is comparable to 2.158 (2)Å found in catena-(tetrakis(μ_2-thiocyanato-N,S)-bis(dimethyl sulfoxide-O)- manganese(II)-mercury(II) (Wang *et al.*, 2000), in which the dimethyl sulfoxide shows a similar terminal η^1-coordinated bonding to the Mn^{II}.

S2. Experimental

$Mn(CH_3CO_2)_2.4H_2O$ (25 mg, 0.1 mmol) was dissolved in 3 ml deionized water with stirring at room temperature. After half an hour, 1 ml dimethyl sulfoxide was added to the solution. The mixed solution was stirred for another half hour, and then filtered. The clear solution obtained was left to stand in the air to let the solvent to evaporate. The colorless crystals were deposited after one week (12.60 mg, yield 56%).

S3. Refinement

An absolute structure was determined using the Flack (1983) method. The hydrogen atoms were placed in idealized positions and allowed to ride on the parent carbon atoms, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C).

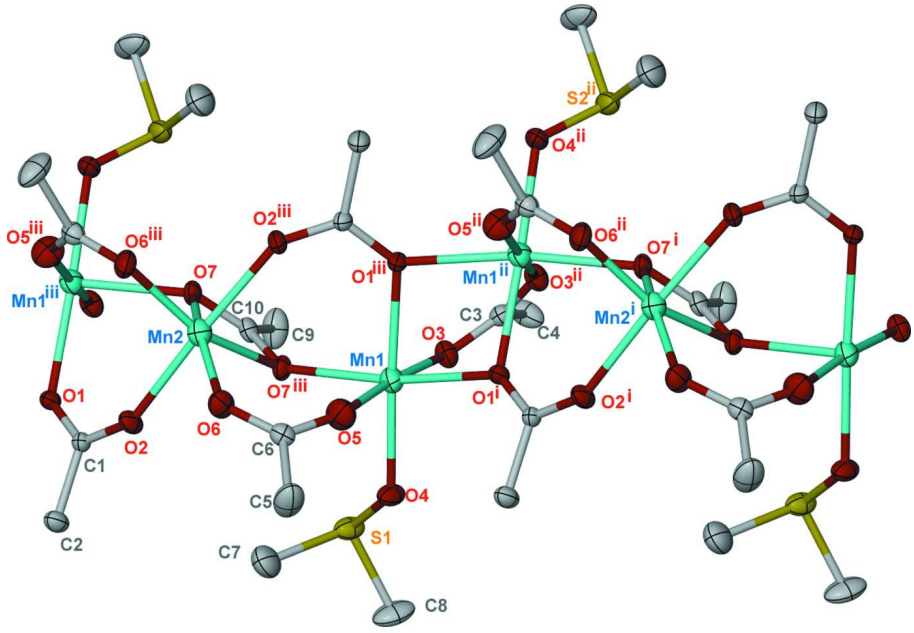

Figure 1

A view of the title complex with the atom-numbering scheme; hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn at 30% probability level. Symmetry codes: i *x*, *y*, *z*-1; ii -*x*+2,*y*,-*z*; iii -*x* + 2, *y*, -*z* +1.

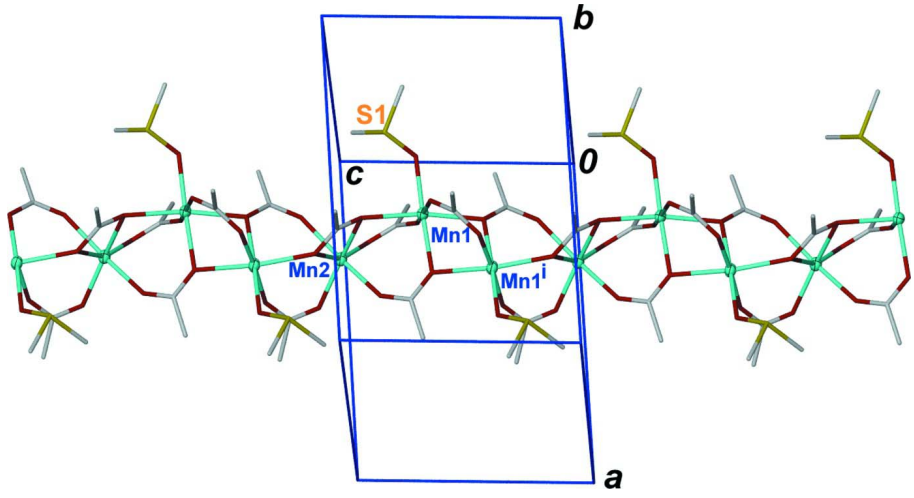

Figure 2

Infinite chain of the Mn^{II} ions bridged by acetate anions along the *c* direction in a unit cell. Symmetry code: i -*x* + 2, *y*, -*z*.

Poly[hexa-*μ*-acetato-bis(dimethyl sulfoxide)trimanganese(II)]

Crystal data

$[Mn_3(C_2H_3O_2)_6(C_2H_6OS)_2]$
M_r = 675.34
Monoclinic, *C*2
Hall symbol: C 2y
a = 12.8475 (16) Å
b = 12.5439 (16) Å
c = 8.6095 (11) Å
β = 94.906 (2)°
V = 1382.4 (3) Å^3
Z = 2
F(000) = 690
D_x = 1.622 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
θ = 2.4–25.1°

μ = 1.56 mm^{-1}
T = 293 K

Block, colorless
0.41 × 0.36 × 0.29 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.883, T_{max} = 1.000

3821 measured reflections
1953 independent reflections
1919 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.1°, θ_{min} = 2.4°
h = −15→15
k = −12→14
l = −10→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.056
S = 1.05
1953 reflections
161 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.3155P]$ $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 653 Friedel pairs
Absolute structure parameter: 0.034 (17)

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 $F^2 > 2$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. An absolute structure was established with the Flack parameter of 0.034 (17).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Mn1	0.91731 (2)	0.56819 (3)	0.13931 (4)	0.02995 (11)	
Mn2	1.0000	0.43103 (4)	0.5000	0.03045 (14)	
S1	0.70961 (5)	0.67013 (7)	0.27681 (10)	0.0504 (2)	
O1	0.91650 (12)	0.53278 (16)	0.88461 (19)	0.0352 (4)	
O2	0.87911 (14)	0.44946 (19)	0.6590 (2)	0.0447 (5)	
O3	0.94917 (16)	0.73193 (16)	0.0982 (2)	0.0446 (5)	
O4	0.75455 (15)	0.6046 (2)	0.1528 (2)	0.0526 (6)	
O5	0.87347 (19)	0.4057 (2)	0.1696 (3)	0.0641 (6)	
O6	0.89783 (16)	0.3166 (2)	0.3901 (2)	0.0517 (5)	
O7	1.05675 (14)	0.59438 (15)	0.60213 (19)	0.0379 (4)	
C1	0.85462 (19)	0.4827 (2)	0.7865 (3)	0.0318 (5)	

C2	0.7442 (2)	0.4630 (3)	0.8279 (4)	0.0454 (7)	
H2A	0.7355	0.4928	0.9287	0.068*	
H2B	0.7312	0.3877	0.8299	0.068*	
H2C	0.6958	0.4961	0.7515	0.068*	
C3	1.0000	0.7770 (3)	0.0000	0.0376 (8)	
C4	1.0000	0.8965 (4)	0.0000	0.0634 (14)	
H4A	1.0425	0.9220	−0.0786	0.095*	0.50
H4B	1.0277	0.9220	0.1003	0.095*	0.50
H4C	0.9298	0.9220	−0.0217	0.095*	0.50
C5	0.7587 (3)	0.2664 (4)	0.2103 (5)	0.0792 (13)	
H5A	0.7291	0.2898	0.1099	0.119*	
H5B	0.7069	0.2712	0.2841	0.119*	
H5C	0.7814	0.1937	0.2033	0.119*	
C6	0.8501 (2)	0.3355 (2)	0.2627 (3)	0.0386 (6)	
C7	0.6698 (3)	0.5766 (5)	0.4144 (5)	0.0873 (14)	
H7A	0.7303	0.5483	0.4736	0.131*	
H7B	0.6320	0.5197	0.3607	0.131*	
H7C	0.6257	0.6113	0.4834	0.131*	
C8	0.5846 (3)	0.7060 (4)	0.1907 (5)	0.0799 (13)	
H8A	0.5918	0.7598	0.1130	0.120*	
H8B	0.5432	0.7333	0.2694	0.120*	
H8C	0.5511	0.6444	0.1429	0.120*	
C9	1.0000	0.7628 (4)	0.5000	0.0727 (16)	
H9A	0.9531	0.7883	0.4154	0.109*	0.50
H9B	1.0693	0.7883	0.4878	0.109*	0.50
H9C	0.9776	0.7883	0.5969	0.109*	0.50
C10	1.0000	0.6450 (4)	0.5000	0.0383 (9)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.02796 (17)	0.0394 (2)	0.02291 (18)	0.00325 (16)	0.00453 (12)	0.00263 (16)
Mn2	0.0318 (3)	0.0360 (3)	0.0238 (3)	0.000	0.00371 (19)	0.000
S1	0.0378 (4)	0.0585 (5)	0.0547 (5)	0.0060 (3)	0.0025 (3)	−0.0202 (4)
O1	0.0278 (8)	0.0502 (11)	0.0278 (9)	−0.0062 (8)	0.0037 (7)	−0.0038 (8)
O2	0.0401 (9)	0.0648 (14)	0.0305 (9)	−0.0086 (9)	0.0107 (8)	−0.0127 (9)
O3	0.0549 (11)	0.0398 (11)	0.0407 (11)	0.0029 (9)	0.0141 (9)	0.0029 (8)
O4	0.0341 (10)	0.0810 (17)	0.0428 (11)	0.0108 (9)	0.0043 (8)	−0.0150 (11)
O5	0.0691 (15)	0.0525 (15)	0.0704 (16)	−0.0129 (12)	0.0037 (12)	0.0102 (12)
O6	0.0554 (11)	0.0611 (14)	0.0382 (11)	−0.0123 (10)	0.0010 (9)	−0.0110 (10)
O7	0.0454 (9)	0.0452 (12)	0.0229 (8)	−0.0039 (8)	0.0019 (7)	0.0009 (8)
C1	0.0285 (12)	0.0419 (14)	0.0248 (12)	−0.0027 (10)	0.0020 (10)	0.0013 (11)
C2	0.0345 (13)	0.065 (2)	0.0369 (15)	−0.0113 (13)	0.0062 (11)	−0.0079 (13)
C3	0.0337 (17)	0.039 (2)	0.040 (2)	0.000	−0.0017 (15)	0.000
C4	0.061 (3)	0.041 (2)	0.092 (4)	0.000	0.031 (3)	0.000
C5	0.078 (2)	0.087 (3)	0.068 (2)	−0.039 (2)	−0.020 (2)	0.009 (2)
C6	0.0384 (13)	0.0347 (14)	0.0433 (15)	−0.0019 (11)	0.0079 (11)	−0.0041 (12)
C7	0.076 (2)	0.134 (4)	0.054 (2)	−0.005 (3)	0.0194 (18)	0.000 (3)

C8	0.0454 (17)	0.081 (3)	0.110 (3)	0.0282 (19)	−0.0133 (19)	−0.029 (3)
C9	0.120 (5)	0.046 (3)	0.051 (3)	0.000	0.000 (3)	0.000
C10	0.047 (2)	0.043 (2)	0.0272 (19)	0.000	0.0116 (17)	0.000

Geometric parameters (Å, º)

Mn1—O3	2.130 (2)	C1—C2	1.513 (4)
Mn1—O5	2.136 (2)	C2—H2A	0.9600
Mn1—O4	2.1533 (19)	C2—H2B	0.9600
Mn1—O1^{i}	2.2076 (15)	C2—H2C	0.9600
Mn1—O1^{ii}	2.2365 (17)	C3—O3^{iv}	1.247 (3)
Mn1—O7^{i}	2.2467 (17)	C3—C4	1.498 (6)
Mn2—O6	2.113 (2)	C4—H4A	0.9600
Mn2—O6^{i}	2.113 (2)	C4—H4B	0.9600
Mn2—O2	2.1690 (18)	C4—H4C	0.9600
Mn2—O2^{i}	2.1690 (18)	C5—C6	1.499 (5)
Mn2—O7	2.3224 (19)	C5—H5A	0.9600
Mn2—O7^{i}	2.3224 (19)	C5—H5B	0.9600
S1—O4	1.501 (2)	C5—H5C	0.9600
S1—C8	1.768 (3)	C7—H7A	0.9600
S1—C7	1.773 (5)	C7—H7B	0.9600
O1—C1	1.275 (3)	C7—H7C	0.9600
O1—Mn1^{i}	2.2076 (15)	C8—H8A	0.9600
O1—Mn1^{iii}	2.2365 (17)	C8—H8B	0.9600
O2—C1	1.239 (3)	C8—H8C	0.9600
O3—C3	1.247 (3)	C9—C10	1.477 (7)
O5—C6	1.245 (4)	C9—H9A	0.9600
O6—C6	1.233 (4)	C9—H9B	0.9600
O7—C10	1.264 (3)	C9—H9C	0.9600
O7—Mn1^{i}	2.2467 (17)	C10—O7^{i}	1.264 (3)
O3—Mn1—O5	175.34 (9)	O1—C1—C2	117.9 (2)
O3—Mn1—O4	90.32 (9)	C1—C2—H2A	109.5
O5—Mn1—O4	85.91 (10)	C1—C2—H2B	109.5
O3—Mn1—O1^{i}	88.70 (8)	H2A—C2—H2B	109.5
O5—Mn1—O1^{i}	94.97 (9)	C1—C2—H2C	109.5
O4—Mn1—O1^{i}	177.66 (7)	H2A—C2—H2C	109.5
O3—Mn1—O1^{ii}	90.78 (7)	H2B—C2—H2C	109.5
O5—Mn1—O1^{ii}	87.19 (9)	O3^{iv}—C3—O3	126.1 (4)
O4—Mn1—O1^{ii}	99.89 (7)	O3^{iv}—C3—C4	116.97 (19)
O1^{i}—Mn1—O1^{ii}	78.00 (7)	O3—C3—C4	116.97 (19)
O3—Mn1—O7^{i}	90.53 (7)	C3—C4—H4A	109.5
O5—Mn1—O7^{i}	92.12 (9)	C3—C4—H4B	109.5
O4—Mn1—O7^{i}	88.74 (7)	H4A—C4—H4B	109.5
O1^{i}—Mn1—O7^{i}	93.39 (6)	C3—C4—H4C	109.5
O1^{ii}—Mn1—O7^{i}	171.26 (6)	H4A—C4—H4C	109.5
O6—Mn2—O6^{i}	94.44 (13)	H4B—C4—H4C	109.5
O6—Mn2—O2	84.50 (8)	C6—C5—H5A	109.5

O6^{i}—Mn2—O2	103.92 (8)	C6—C5—H5B	109.5
O6—Mn2—O2^{i}	103.92 (8)	H5A—C5—H5B	109.5
O6^{i}—Mn2—O2^{i}	84.50 (8)	C6—C5—H5C	109.5
O2—Mn2—O2^{i}	167.76 (13)	H5A—C5—H5C	109.5
O6—Mn2—O7	158.69 (8)	H5B—C5—H5C	109.5
O6^{i}—Mn2—O7	105.48 (8)	O6—C6—O5	125.5 (3)
O2—Mn2—O7	83.42 (7)	O6—C6—C5	118.3 (3)
O2^{i}—Mn2—O7	85.78 (8)	O5—C6—C5	116.2 (3)
O6—Mn2—O7^{i}	105.48 (8)	S1—C7—H7A	109.5
O6^{i}—Mn2—O7^{i}	158.69 (8)	S1—C7—H7B	109.5
O2—Mn2—O7^{i}	85.78 (8)	H7A—C7—H7B	109.5
O2^{i}—Mn2—O7^{i}	83.42 (7)	S1—C7—H7C	109.5
O7—Mn2—O7^{i}	56.16 (9)	H7A—C7—H7C	109.5
O4—S1—C8	103.40 (16)	H7B—C7—H7C	109.5
O4—S1—C7	105.3 (2)	S1—C8—H8A	109.5
C8—S1—C7	98.3 (2)	S1—C8—H8B	109.5
C1—O1—Mn1^{i}	126.19 (15)	H8A—C8—H8B	109.5
C1—O1—Mn1^{iii}	134.27 (15)	S1—C8—H8C	109.5
Mn1^{i}—O1—Mn1^{iii}	97.36 (6)	H8A—C8—H8C	109.5
C1—O2—Mn2	147.63 (17)	H8B—C8—H8C	109.5
C3—O3—Mn1	132.0 (2)	C10—C9—H9A	109.5
S1—O4—Mn1	126.07 (12)	C10—C9—H9B	109.5
C6—O5—Mn1	146.5 (2)	H9A—C9—H9B	109.5
C6—O6—Mn2	120.7 (2)	C10—C9—H9C	109.5
C10—O7—Mn1^{i}	142.22 (15)	H9A—C9—H9C	109.5
C10—O7—Mn2	92.1 (2)	H9B—C9—H9C	109.5
Mn1^{i}—O7—Mn2	105.15 (7)	O7^{i}—C10—O7	119.7 (4)
O2—C1—O1	124.1 (2)	O7^{i}—C10—C9	120.16 (19)
O2—C1—C2	117.9 (2)	O7—C10—C9	120.16 (19)

O6—Mn2—O2—C1	163.4 (4)	O6—Mn2—O7—C10	−33.4 (2)
O6^{i}—Mn2—O2—C1	70.2 (4)	O6^{i}—Mn2—O7—C10	168.01 (9)
O2^{i}—Mn2—O2—C1	−62.4 (4)	O2—Mn2—O7—C10	−89.32 (10)
O7—Mn2—O2—C1	−34.2 (4)	O2^{i}—Mn2—O7—C10	84.91 (9)
O7^{i}—Mn2—O2—C1	−90.5 (4)	O7^{i}—Mn2—O7—C10	0.0
O5—Mn1—O3—C3	−96.9 (11)	O6—Mn2—O7—Mn1^{i}	112.59 (19)
O4—Mn1—O3—C3	−132.66 (18)	O6^{i}—Mn2—O7—Mn1^{i}	−45.97 (9)
O1^{i}—Mn1—O3—C3	45.22 (18)	O2—Mn2—O7—Mn1^{i}	56.70 (8)
O1^{ii}—Mn1—O3—C3	−32.76 (18)	O2^{i}—Mn2—O7—Mn1^{i}	−129.08 (8)
O7^{i}—Mn1—O3—C3	138.60 (19)	O7^{i}—Mn2—O7—Mn1^{i}	146.02 (13)
C8—S1—O4—Mn1	161.6 (2)	Mn2—O2—C1—O1	2.3 (6)
C7—S1—O4—Mn1	−95.7 (2)	Mn2—O2—C1—C2	−177.9 (3)
O3—Mn1—O4—S1	−66.55 (18)	Mn1^{i}—O1—C1—O2	−2.6 (4)
O5—Mn1—O4—S1	116.18 (19)	Mn1^{iii}—O1—C1—O2	−161.7 (2)
O1^{i}—Mn1—O4—S1	−132 (2)	Mn1^{i}—O1—C1—C2	177.7 (2)
O1^{ii}—Mn1—O4—S1	−157.39 (17)	Mn1^{iii}—O1—C1—C2	18.5 (4)
O7^{i}—Mn1—O4—S1	23.97 (18)	Mn1—O3—C3—O3^{iv}	−3.74 (11)
O3—Mn1—O5—C6	−114.0 (11)	Mn1—O3—C3—C4	176.26 (11)

O4—Mn1—O5—C6	−78.1 (4)	Mn2—O6—C6—O5	18.9 (4)
O1^{i}—Mn1—O5—C6	104.1 (4)	Mn2—O6—C6—C5	−163.8 (3)
O1^{ii}—Mn1—O5—C6	−178.2 (4)	Mn1—O5—C6—O6	−46.7 (6)
O7^{i}—Mn1—O5—C6	10.5 (4)	Mn1—O5—C6—C5	135.9 (4)
O6^{i}—Mn2—O6—C6	−148.6 (2)	Mn1^{i}—O7—C10—O7^{i}	−118.3 (3)
O2—Mn2—O6—C6	107.8 (2)	Mn2—O7—C10—O7^{i}	0.0
O2^{i}—Mn2—O6—C6	−63.2 (2)	Mn1^{i}—O7—C10—C9	61.7 (3)
O7—Mn2—O6—C6	52.1 (3)	Mn2—O7—C10—C9	180.0
O7^{i}—Mn2—O6—C6	23.7 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···O6^{v}	0.96	2.45	3.367 (4)	160
C2—H2*B*···S1^{vi}	0.96	2.99	3.841 (4)	147

Symmetry codes: (v) *x*−1/2, *y*+1/2, *z*; (vi) −*x*+3/2, *y*−1/2, −*z*+1.