Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

μ_3-Oxo-hexa-μ_2-pivalato-(pivalic acid-κO)-bis(pyridine-κN)trimanganese(III,III,II)

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.008 Å
Disorder in main residue
R factor = 0.057
wR factor = 0.135
Data-to-parameter ratio = 16.5

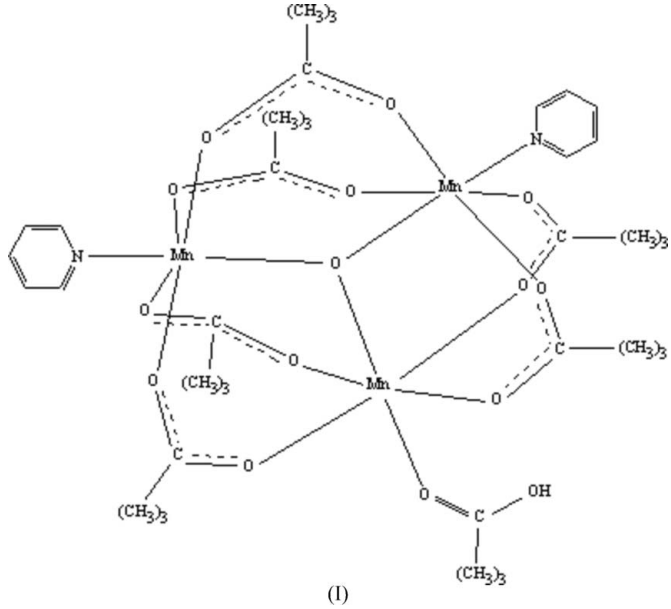
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 27 September 2006
Accepted 13 November 2006

The asymmetric unit of the title compound, $[Mn_3(C_5H_9O_2)_6O(C_5H_5N)_2(C_5H_{10}O_2)]$, comprises two independent and similar $[Mn^{III}_2Mn^{II}O\{(CH_3)_3CCO_2\}_6(py)_2(CH_3)_3CCOOH]$ (py = pyridine) molecules each with an $Mn_3(\mu_3\text{-}O)$ core. In each molecule, the Mn atoms have octahedral geometry with two coordinated pyridines bonded to two Mn^{III} and a terminal pivalic acid coordinated to the Mn^{II} atom.

Comment

Oxo-centered triangular Mn complexes, $Mn_3(\mu_3\text{-}O)$, have been considered as effective models for studying *M–M* interactions in mixed-metal clusters, and electron delocalization in mixed-valence clusters. A wide variety of mixed-metal combinations and mixed-valency combinations have been reported (Cannon & White, 1988; Jayasooriya *et al.*, 1989; Wu *et al.*, 1998). In the $Mn_3(\mu_3\text{-}O)$ systems, the geometry of the central core remains relatively constant throughout the series and is often close to having threefold symmetry with a planar M_3O unit (Wu *et al.*, 1998).



(I)

In (I), the three Mn atoms form a regular triangular geometry and are linked by a central μ_3-O atom (Fig. 1). The asymmetric unit consists of two independent and similar molecules (*A* and *B*), $[Mn^{III}_2Mn^{II}O\{(CH_3)_3CCO_2\}_6(py)_2(CH_3)_3CCO$-

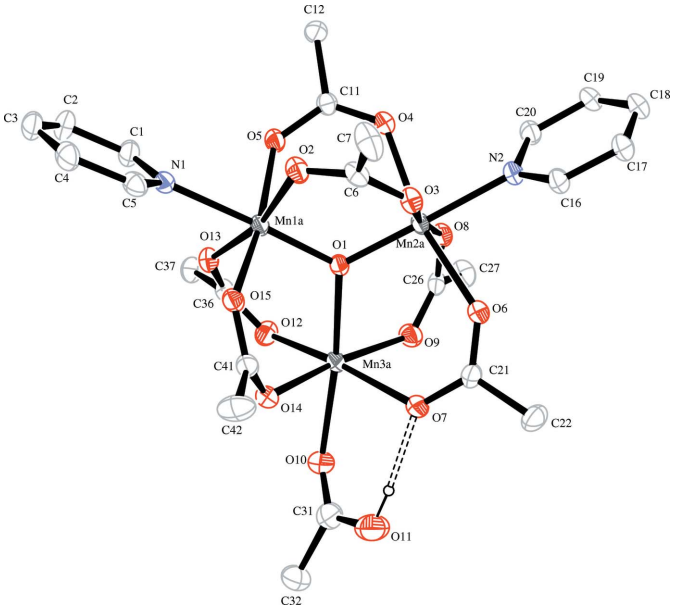


Figure 1
The molecular structure and atomic labelling scheme of molecule *A* in (I). Displacement ellipsoids are drawn at the 20% probability level. The *tert*-butyl methyl groups and H atoms, except for those of the pivalic acid ligands, have been omitted for clarity and open dashed lines indicate hydrogen bonds.

OH]. The Mn atoms in both molecules have two different types of Mn—(μ_3-O) bond lengths (Table 1). The Mn_3 triangle is isosceles and clearly indicates that one Mn atom differs from the other two. This is most logically interpreted in terms of identifying Mn3*A* and Mn3*B* as having different oxidation states from the other Mn atoms. This asymmetry is most noticeable in the Mn_3O central core, with longer Mn3*A*—O1 and Mn3*B*—O16 distances.

The planes of the coordinated pyridines are almost orthogonal to the central Mn_3O core. The Mn—N bond lengths in *A* and *B* are quite similar and in the range 2.081 (3) to 2.094 (4) Å: these bond lengths agree with Mn^{III}—N for related $Mn_3(\mu_3$-O) complexes [2.061 (10)–2.280 (7) Å; Baikie *et al.*, 1978; Baikie *et al.*, 1980; Vincent *et al.*, 1987; Wu *et al.*, 1998]. Other selected bond lengths and angles agree well with the literature values (see previous references).

In both molecules, the Mn^{III} atoms show a typical Jahn–Teller distortion, with two longer and two shorter Mn—O bonds. The long pair form a long axis in a pseudo-octahedral coordination (Wu *et al.*, 1998). The crystal structure is stabilized by intermolecular O—H···O hydrogen bonds involving the H atoms of terminal pivalic acid groups and O atoms of the pivalate groups (Table 2).

Experimental

A mixture of molten pivalic acid (60 ml), pyridine (40 ml) and water (20 ml) was added to a mixture of ground $MnCl_2{\cdot}4H_2O$ (8.8 g, 44 mmol) and finely ground $KMnO_4$ (0.81 g, 5.2 mmol) in a 250 ml conical flask. The mixture was heated at 323–333 K with stirring and then the mixture was left to cool and filtered. Two layers in the flask were separated and after several days black crystals from the organic layer were collected, washed thoroughly with water and dried in air.

Crystal data

$[Mn_3(C_5H_9O_2)_6O(C_5H_5N)_2(C_5H_{10}O_2)]$
M_r = 1047.88
Monoclinic, $P2_1/c$
a = 27.1668 (7) Å
b = 19.3139 (4) Å
c = 22.8444 (5) Å
β = 109.361 (2)°
V = 11308.5 (5) Å^3
Z = 8
D_x = 1.231 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 150 (2) K
Prism, black
0.52 × 0.32 × 0.22 mm

Data collection

Stoe IDPS-2 diffractometer
Rotation method scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.759, T_{max} = 0.854
20095 measured reflections
19951 independent reflections
12017 reflections with $I > 2\sigma(I)$
R_{int} = 0.110
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.123
S = 1.05
19951 reflections
1220 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.024
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: none

Table 1
Selected geometric parameters (Å, °).

Mn1*A*—O1	1.810 (3)	Mn1*B*—O16	1.818 (3)
Mn1*A*—O2	2.140 (3)	Mn1*B*—O17	2.198 (3)
Mn1*A*—O5	2.004 (3)	Mn1*B*—O19	1.967 (3)
Mn1*A*—O13	2.076 (3)	Mn1*B*—O28	1.962 (3)
Mn1*A*—O15	2.008 (3)	Mn1*B*—O30	2.119 (3)
Mn2*A*—O1	1.814 (3)	Mn2*B*—O16	1.816 (3)
Mn2*A*—O3	1.978 (3)	Mn2*B*—O18	1.966 (3)
Mn2*A*—O4	2.167 (3)	Mn2*B*—O20	2.162 (3)
Mn2*A*—O6	2.145 (3)	Mn2*B*—O21	1.960 (3)
Mn2*A*—O8	1.960 (3)	Mn2*B*—O23	2.174 (3)
Mn3*A*—O1	2.124 (3)	Mn3*B*—O16	2.109 (3)
Mn3*A*—O7	2.207 (3)	Mn3*B*—O22	2.133 (3)
Mn3*A*—O9	2.130 (3)	Mn3*B*—O24	2.221 (3)
Mn3*A*—O10	2.224 (4)	Mn3*B*—O25	2.251 (3)
Mn3*A*—O12	2.129 (4)	Mn3*B*—O27	2.177 (3)
Mn3*A*—O14	2.169 (3)	Mn3*B*—O29	2.131 (3)
O1—Mn1*A*—N1	177.67 (13)	O16—Mn1*B*—N3	178.90 (14)
O1—Mn2*A*—N2	178.47 (15)	O16—Mn2*B*—N4	176.27 (14)
Mn1*A*—O1—Mn2*A*	122.36 (15)	Mn1*B*—O16—Mn2*B*	124.60 (15)
Mn1*A*—O1—Mn3*A*	118.09 (14)	Mn1*B*—O16—Mn3*B*	115.50 (13)
Mn2*A*—O1—Mn3*A*	119.55 (14)	Mn2*B*—O16—Mn3*B*	119.88 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H11···O7	0.84	1.77	2.605 (5)	172
O26—H26···O24	0.84	1.73	2.560 (4)	170

Ten *tert*-butyl groups are disordered, giving unrealistically anisotropic displacement parameters and bond lengths. The refinement was performed with soft restraints for the split C atom sites, leading to

satisfactory refinement results. For the disordered *tert*-butyl groups the C—CH_3 distances were constrained to 1.52 (2) Å. Fixed occupancy factors of 0.5 were applied for both positions initially as it was possible to obtain reasonable refined values for related pairs: these were subsequently allowed to vary but constrained to sum to unit occupancy. All non-H atoms, except for the disordered C atoms, were assigned anisotropic displacement parameters. The H atoms were placed in idealized positions and refined using a riding model, with distances in the range 0.84–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C,O) or 1.5U_{eq}(methyl C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for use of the Stoe IPDS2 diffractometer purchased under grant F.279 of the University Research Fund and also thank Gazi University Scientific Research Unit (BAP-04/2004–12) for financial support for this study.

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supporting information

Acta Cryst. (2006). E**62**, m3439–m3441 [https://doi.org/10.1107/S1600536806048343]

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Crystal data

$[Mn_3(C_5H_9O_2)_6O(C_5H_5N)_2(C_5H_{10}O_2)]$
$M_r = 1047.88$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 27.1668$ (7) Å
$b = 19.3139$ (4) Å
$c = 22.8444$ (5) Å
$\beta = 109.361$ (2)°
$V = 11308.5$ (5) Å^3
$Z = 8$
$F(000) = 4424$
$D_x = 1.231$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 1.3$–$25.1°$
$\mu = 0.72$ mm^{-1}
$T = 150$ K
Prism, black
0.52 × 0.32 × 0.22 mm

Data collection

Stoe IPDS-2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
φ? ω? scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{min} = 0.759$, $T_{max} = 0.854$
20095 measured reflections
19951 independent reflections
12017 reflections with $I > 2\sigma(I)$
$R_{int} = 0.110$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.3°$
$h = -32 \rightarrow 32$
$k = -23 \rightarrow 23$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.123$
$S = 1.05$
19951 reflections
1220 parameters
171 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
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.024$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}
Extinction correction: SHELXL97
Extinction coefficient: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mn1A	0.82531 (3)	0.29243 (3)	0.28979 (3)	0.03915 (16)	
Mn2A	0.86849 (3)	0.22251 (3)	0.19076 (3)	0.04138 (16)	
Mn3A	0.92477 (3)	0.17895 (4)	0.34288 (3)	0.04764 (18)	
O1	0.86982 (11)	0.23465 (14)	0.27000 (12)	0.0407 (7)	
O2	0.82317 (13)	0.36962 (15)	0.22181 (14)	0.0527 (8)	
O3	0.87468 (13)	0.32199 (16)	0.17391 (13)	0.0510 (8)	
O4	0.78475 (13)	0.23235 (16)	0.14760 (13)	0.0508 (8)	
O5	0.75918 (12)	0.25502 (16)	0.22926 (13)	0.0495 (8)	
O6	0.95130 (13)	0.21480 (17)	0.21140 (14)	0.0553 (8)	
O7	0.99221 (12)	0.20329 (19)	0.31305 (14)	0.0614 (9)	
O8	0.86048 (12)	0.12173 (16)	0.19245 (13)	0.0503 (8)	
O9	0.91518 (14)	0.08968 (17)	0.28545 (15)	0.0592 (9)	
O10	0.98269 (16)	0.1329 (2)	0.42685 (17)	0.0720 (10)	
O11	1.05629 (18)	0.1799 (3)	0.4246 (2)	0.1142 (17)	
H11	1.0378	0.1903	0.3883	0.171*	
O12	0.86718 (14)	0.13979 (17)	0.37859 (15)	0.0594 (9)	
O13	0.81207 (12)	0.22856 (15)	0.35614 (14)	0.0481 (7)	
O14	0.94451 (12)	0.27384 (17)	0.39639 (14)	0.0536 (8)	
O15	0.88333 (12)	0.35050 (15)	0.34550 (13)	0.0470 (7)	
N1	0.77634 (15)	0.35958 (18)	0.31612 (15)	0.0454 (9)	
N2	0.86506 (15)	0.20725 (19)	0.09931 (16)	0.0473 (9)	
C1	0.7333 (2)	0.3357 (3)	0.3248 (2)	0.0574 (13)	
H1	0.7249	0.2880	0.3178	0.069*	
C2	0.7005 (2)	0.3779 (3)	0.3437 (3)	0.0721 (16)	
H2	0.6702	0.3591	0.3497	0.087*	
C3	0.7115 (3)	0.4463 (3)	0.3538 (2)	0.0711 (16)	
H3	0.6891	0.4762	0.3665	0.085*	
C4	0.7557 (3)	0.4709 (3)	0.3453 (2)	0.0703 (16)	
H4	0.7650	0.5183	0.3528	0.084*	
C5	0.7871 (2)	0.4266 (2)	0.3258 (2)	0.0550 (13)	
H5	0.8173	0.4446	0.3192	0.066*	
C6	0.8500 (2)	0.3732 (2)	0.1867 (2)	0.0529 (12)	
C7	0.8506 (2)	0.4412 (2)	0.1537 (2)	0.0777 (18)	
C8A	0.8490 (6)	0.5021 (5)	0.1936 (5)	0.079 (5)*	0.559 (15)
H8A	0.8513	0.5450	0.1717	0.118*	0.559 (15)
H8B	0.8785	0.4996	0.2325	0.118*	0.559 (15)
H8C	0.8162	0.5016	0.2027	0.118*	0.559 (15)
C9A	0.7958 (4)	0.4385 (6)	0.0977 (5)	0.074 (4)*	0.559 (15)
H9A	0.7913	0.4810	0.0731	0.111*	0.559 (15)
H9B	0.7672	0.4343	0.1148	0.111*	0.559 (15)
H9C	0.7954	0.3985	0.0713	0.111*	0.559 (15)
C10A	0.8902 (5)	0.4452 (7)	0.1230 (7)	0.099 (5)*	0.559 (15)
H10A	0.8865	0.4054	0.0953	0.148*	0.559 (15)
H10B	0.9250	0.4448	0.1544	0.148*	0.559 (15)
H10C	0.8854	0.4881	0.0989	0.148*	0.559 (15)

C8C	0.8324 (6)	0.5005 (5)	0.1857 (6)	0.053 (4)*	0.441 (15)
H8D	0.8348	0.5442	0.1651	0.080*	0.441 (15)
H8E	0.8545	0.5027	0.2293	0.080*	0.441 (15)
H8F	0.7961	0.4925	0.1831	0.080*	0.441 (15)
C9C	0.8264 (7)	0.4360 (8)	0.0866 (4)	0.102 (6)*	0.441 (15)
H9D	0.8270	0.4815	0.0677	0.153*	0.441 (15)
H9E	0.7902	0.4206	0.0767	0.153*	0.441 (15)
H9F	0.8456	0.4026	0.0703	0.153*	0.441 (15)
C10C	0.9106 (4)	0.4554 (8)	0.1645 (8)	0.089 (5)*	0.441 (15)
H10D	0.9237	0.4207	0.1422	0.134*	0.441 (15)
H10E	0.9303	0.4527	0.2090	0.134*	0.441 (15)
H10F	0.9146	0.5017	0.1491	0.134*	0.441 (15)
C11	0.75036 (19)	0.2439 (2)	0.1714 (2)	0.0472 (11)	
C12	0.69318 (19)	0.2456 (3)	0.1309 (2)	0.0600 (13)	
C13	0.6670 (2)	0.1829 (4)	0.1471 (3)	0.094 (2)	
H13A	0.6304	0.1814	0.1203	0.141*	
H13B	0.6688	0.1859	0.1906	0.141*	
H13C	0.6848	0.1408	0.1409	0.141*	
C14	0.6687 (2)	0.3131 (4)	0.1438 (3)	0.096 (2)	
H14A	0.6316	0.3141	0.1189	0.144*	
H14B	0.6864	0.3527	0.1329	0.144*	
H14C	0.6724	0.3154	0.1879	0.144*	
C15	0.6882 (2)	0.2426 (4)	0.0626 (2)	0.0845 (19)	
H15A	0.6512	0.2410	0.0372	0.127*	
H15B	0.7059	0.2011	0.0548	0.127*	
H15C	0.7044	0.2838	0.0517	0.127*	
C16	0.8964 (2)	0.2420 (3)	0.0750 (2)	0.0525 (12)	
H16	0.9205	0.2744	0.1001	0.063*	
C17	0.8945 (2)	0.2318 (3)	0.0145 (2)	0.0630 (14)	
H17	0.9168	0.2574	−0.0019	0.076*	
C18	0.8601 (2)	0.1845 (3)	−0.0216 (2)	0.0660 (15)	
H18	0.8589	0.1761	−0.0630	0.079*	
C19	0.8273 (2)	0.1493 (3)	0.0026 (2)	0.0610 (14)	
H19	0.8026	0.1172	−0.0221	0.073*	
C20	0.8309 (2)	0.1616 (3)	0.0630 (2)	0.0538 (12)	
H20	0.8085	0.1370	0.0799	0.065*	
C21	0.99165 (18)	0.2084 (3)	0.2574 (2)	0.0527 (12)	
C22	1.0419 (2)	0.2027 (3)	0.2441 (2)	0.0775 (17)	
C23A	1.0465 (4)	0.2567 (5)	0.1991 (4)	0.073 (3)*	0.603 (11)
H23A	1.0437	0.3028	0.2157	0.109*	0.603 (11)
H23B	1.0185	0.2505	0.1594	0.109*	0.603 (11)
H23C	1.0804	0.2522	0.1929	0.109*	0.603 (11)
C24A	1.0894 (3)	0.1935 (6)	0.2981 (4)	0.086 (4)*	0.603 (11)
H24A	1.1190	0.1839	0.2839	0.129*	0.603 (11)
H24B	1.0846	0.1547	0.3233	0.129*	0.603 (11)
H24C	1.0963	0.2359	0.3232	0.129*	0.603 (11)
C25A	1.0361 (4)	0.1300 (4)	0.2081 (5)	0.094 (4)*	0.603 (11)
H25A	1.0685	0.1195	0.2000	0.141*	0.603 (11)

H25B	1.0072	0.1329	0.1687	0.141*	0.603 (11)
H25C	1.0289	0.0932	0.2337	0.141*	0.603 (11)
C23C	1.0392 (7)	0.2266 (10)	0.1811 (5)	0.100 (6)*	0.397 (11)
H23D	1.0235	0.2728	0.1735	0.150*	0.397 (11)
H23E	1.0178	0.1943	0.1499	0.150*	0.397 (11)
H23F	1.0744	0.2284	0.1785	0.150*	0.397 (11)
C24C	1.0772 (7)	0.2602 (9)	0.2897 (8)	0.132 (9)*	0.397 (11)
H24D	1.0647	0.2673	0.3248	0.197*	0.397 (11)
H24E	1.0750	0.3038	0.2671	0.197*	0.397 (11)
H24F	1.1136	0.2445	0.3051	0.197*	0.397 (11)
C25C	1.0724 (7)	0.1392 (7)	0.2694 (9)	0.124 (8)*	0.397 (11)
H25D	1.1073	0.1432	0.2659	0.186*	0.397 (11)
H25E	1.0545	0.0988	0.2459	0.186*	0.397 (11)
H25F	1.0755	0.1338	0.3132	0.186*	0.397 (11)
C26	0.88364 (19)	0.0761 (2)	0.2333 (2)	0.0488 (11)	
C27	0.8702 (2)	0.0014 (3)	0.2147 (2)	0.0680 (15)	
C28A	0.9032 (6)	−0.0478 (7)	0.2591 (7)	0.124 (5)*	0.677 (11)
H28A	0.9391	−0.0442	0.2589	0.186*	0.677 (11)
H28B	0.8903	−0.0949	0.2474	0.186*	0.677 (11)
H28C	0.9023	−0.0374	0.3007	0.186*	0.677 (11)
C29A	0.8095 (4)	−0.0049 (6)	0.2066 (6)	0.089 (3)*	0.677 (11)
H29A	0.7976	−0.0523	0.1941	0.133*	0.677 (11)
H29B	0.7895	0.0276	0.1747	0.133*	0.677 (11)
H29C	0.8044	0.0059	0.2461	0.133*	0.677 (11)
C30A	0.8715 (5)	−0.0115 (5)	0.1486 (5)	0.080 (3)*	0.677 (11)
H30A	0.9058	0.0013	0.1467	0.120*	0.677 (11)
H30B	0.8446	0.0166	0.1189	0.120*	0.677 (11)
H30C	0.8649	−0.0606	0.1382	0.120*	0.677 (11)
C28C	0.8855 (7)	−0.0441 (7)	0.2733 (5)	0.057 (5)*	0.323 (11)
H28D	0.8774	−0.0926	0.2613	0.086*	0.323 (11)
H28E	0.8659	−0.0294	0.3002	0.086*	0.323 (11)
H28F	0.9230	−0.0394	0.2955	0.086*	0.323 (11)
C29C	0.8128 (4)	−0.0091 (11)	0.1813 (10)	0.097 (8)*	0.323 (11)
H29D	0.8060	−0.0584	0.1718	0.145*	0.323 (11)
H29E	0.8022	0.0175	0.1426	0.145*	0.323 (11)
H29F	0.7930	0.0066	0.2076	0.145*	0.323 (11)
C30C	0.9016 (8)	−0.0193 (9)	0.1740 (9)	0.088 (7)*	0.323 (11)
H30D	0.9389	−0.0176	0.1982	0.133*	0.323 (11)
H30E	0.8942	0.0127	0.1389	0.133*	0.323 (11)
H30F	0.8921	−0.0665	0.1586	0.133*	0.323 (11)
C31	1.0272 (3)	0.1490 (3)	0.4527 (3)	0.0797 (17)	
C32	1.0567 (2)	0.1329 (3)	0.5203 (3)	0.091 (2)	
C33A	1.0174 (4)	0.1018 (8)	0.5482 (5)	0.099 (4)*	0.73 (2)
H33A	0.9904	0.1361	0.5465	0.148*	0.73 (2)
H33B	1.0356	0.0888	0.5915	0.148*	0.73 (2)
H33C	1.0013	0.0606	0.5245	0.148*	0.73 (2)
C34A	1.0965 (5)	0.0781 (6)	0.5211 (5)	0.095 (4)*	0.73 (2)
H34A	1.1226	0.0975	0.5046	0.143*	0.73 (2)

H34B	1.0790	0.0388	0.4954	0.143*	0.73 (2)
H34C	1.1137	0.0624	0.5638	0.143*	0.73 (2)
C35A	1.0848 (4)	0.1981 (4)	0.5517 (4)	0.084 (4)*	0.73 (2)
H35A	1.1042	0.1880	0.5953	0.126*	0.73 (2)
H35B	1.0592	0.2347	0.5492	0.126*	0.73 (2)
H35C	1.1090	0.2134	0.5307	0.126*	0.73 (2)
C33C	1.0190 (7)	0.1349 (17)	0.5567 (7)	0.071 (8)*	0.27 (2)
H33D	1.0387	0.1340	0.6012	0.107*	0.27 (2)
H33E	0.9959	0.0945	0.5458	0.107*	0.27 (2)
H33F	0.9981	0.1773	0.5465	0.107*	0.27 (2)
C34C	1.0757 (17)	0.0585 (11)	0.5227 (13)	0.157 (18)*	0.27 (2)
H34D	1.0788	0.0460	0.4825	0.235*	0.27 (2)
H34E	1.0508	0.0275	0.5321	0.235*	0.27 (2)
H34F	1.1099	0.0542	0.5551	0.235*	0.27 (2)
C35C	1.1010 (13)	0.183 (2)	0.5450 (14)	0.21 (11)*	0.27 (2)
H35D	1.0898	0.2218	0.5656	0.780*	0.27 (2)
H35E	1.1113	0.2013	0.5107	0.780*	0.27 (2)
H35F	1.1307	0.1598	0.5749	0.780*	0.27 (2)
C36	0.8247 (2)	0.1671 (3)	0.3751 (2)	0.0497 (11)	
C37	0.7839 (2)	0.1253 (3)	0.3919 (2)	0.0578 (13)	
C38	0.8056 (3)	0.0560 (3)	0.4207 (3)	0.0794 (17)	
H38A	0.7793	0.0318	0.4339	0.119*	
H38B	0.8370	0.0637	0.4567	0.119*	
H38C	0.8145	0.0277	0.3900	0.119*	
C39	0.7377 (2)	0.1139 (3)	0.3322 (3)	0.0742 (16)	
H39A	0.7103	0.0880	0.3417	0.111*	
H39B	0.7494	0.0877	0.3025	0.111*	
H39C	0.7239	0.1588	0.3142	0.111*	
C40	0.7652 (2)	0.1675 (3)	0.4382 (3)	0.0715 (15)	
H40A	0.7370	0.1424	0.4469	0.107*	
H40B	0.7524	0.2127	0.4201	0.107*	
H40C	0.7944	0.1740	0.4769	0.107*	
C41	0.92971 (19)	0.3341 (3)	0.3795 (2)	0.0519 (12)	
C42	0.9677 (2)	0.3938 (3)	0.4008 (3)	0.085 (2)	
C43A	0.9463 (5)	0.4630 (4)	0.3799 (6)	0.102 (4)*	0.603 (12)
H43A	0.9161	0.4716	0.3933	0.153*	0.603 (12)
H43B	0.9354	0.4654	0.3345	0.153*	0.603 (12)
H43C	0.9731	0.4981	0.3979	0.153*	0.603 (12)
C44A	0.9881 (5)	0.3901 (7)	0.4735 (4)	0.121 (5)*	0.603 (12)
H44A	0.9599	0.4030	0.4892	0.181*	0.603 (12)
H44B	1.0174	0.4222	0.4898	0.181*	0.603 (12)
H44C	0.9997	0.3429	0.4867	0.181*	0.603 (12)
C45A	1.0174 (4)	0.3749 (7)	0.3874 (7)	0.130 (6)*	0.603 (12)
H45A	1.0449	0.4082	0.4079	0.196*	0.603 (12)
H45B	1.0107	0.3760	0.3425	0.196*	0.603 (12)
H45C	1.0286	0.3283	0.4032	0.196*	0.603 (12)
C43C	0.9406 (7)	0.4542 (8)	0.4203 (10)	0.122 (8)*	0.397 (12)
H43D	0.9268	0.4388	0.4527	0.184*	0.397 (12)

H43E	0.9119	0.4708	0.3844	0.184*	0.397 (12)
H43F	0.9657	0.4917	0.4365	0.184*	0.397 (12)
C44C	1.0183 (5)	0.3756 (10)	0.4470 (8)	0.118 (8)*	0.397 (12)
H44D	1.0402	0.4170	0.4581	0.177*	0.397 (12)
H44E	1.0356	0.3406	0.4297	0.177*	0.397 (12)
H44F	1.0126	0.3570	0.4842	0.177*	0.397 (12)
C45C	0.9763 (8)	0.4163 (11)	0.3396 (7)	0.150 (10)*	0.397 (12)
H45D	0.9996	0.4565	0.3477	0.225*	0.397 (12)
H45E	0.9427	0.4287	0.3087	0.225*	0.397 (12)
H45F	0.9920	0.3781	0.3238	0.225*	0.397 (12)
Mn1B	0.68938 (3)	0.67126 (3)	0.38118 (3)	0.04092 (16)	
Mn2B	0.56915 (2)	0.62799 (3)	0.35102 (3)	0.03668 (15)	
Mn3B	0.60391 (3)	0.79773 (3)	0.37093 (3)	0.04097 (16)	
O16	0.62120 (11)	0.69161 (13)	0.36784 (12)	0.0388 (7)	
O17	0.68762 (12)	0.57536 (15)	0.43229 (13)	0.0465 (7)	
O18	0.60346 (12)	0.57040 (14)	0.42419 (12)	0.0432 (7)	
O19	0.67653 (12)	0.62185 (15)	0.30219 (13)	0.0466 (7)	
O20	0.60129 (12)	0.56872 (14)	0.29198 (13)	0.0442 (7)	
O21	0.52246 (11)	0.67537 (15)	0.27773 (12)	0.0445 (7)	
O22	0.53087 (12)	0.78861 (15)	0.29810 (14)	0.0503 (8)	
O23	0.52823 (11)	0.67380 (15)	0.40869 (13)	0.0437 (7)	
O24	0.56528 (13)	0.77571 (15)	0.44069 (14)	0.0510 (8)	
O25	0.58802 (13)	0.90779 (15)	0.39181 (13)	0.0516 (8)	
O26	0.58384 (15)	0.89755 (16)	0.48677 (15)	0.0609 (9)	
H26	0.5784	0.8560	0.4757	0.091*	
O27	0.67357 (13)	0.81422 (15)	0.45115 (14)	0.0513 (8)	
O28	0.71627 (12)	0.71377 (16)	0.46370 (13)	0.0495 (8)	
O29	0.64217 (13)	0.83526 (16)	0.30949 (14)	0.0521 (8)	
O30	0.70826 (13)	0.76034 (16)	0.33878 (15)	0.0532 (8)	
N3	0.76755 (15)	0.64579 (19)	0.39623 (19)	0.0525 (10)	
N4	0.51211 (14)	0.55075 (17)	0.32912 (15)	0.0427 (9)	
C46	0.7988 (2)	0.6216 (3)	0.4510 (3)	0.0637 (14)	
H46	0.7848	0.6152	0.4836	0.076*	
C47	0.8503 (2)	0.6057 (4)	0.4618 (3)	0.090 (2)	
H47	0.8716	0.5890	0.5012	0.108*	
C48	0.8708 (3)	0.6144 (4)	0.4139 (4)	0.101 (2)	
H48	0.9062	0.6036	0.4198	0.121*	
C49	0.8389 (3)	0.6389 (3)	0.3585 (4)	0.0872 (19)	
H49	0.8519	0.6453	0.3250	0.105*	
C50	0.7876 (2)	0.6544 (3)	0.3510 (3)	0.0657 (14)	
H50	0.7658	0.6718	0.3121	0.079*	
C51	0.65147 (19)	0.5547 (2)	0.45005 (18)	0.0421 (10)	
C52	0.66294 (17)	0.5064 (2)	0.5056 (2)	0.0583 (13)	
C53A	0.6402 (5)	0.5332 (7)	0.5513 (5)	0.085 (4)*	0.509 (13)
H53A	0.6023	0.5382	0.5317	0.127*	0.509 (13)
H53B	0.6555	0.5784	0.5664	0.127*	0.509 (13)
H53C	0.6475	0.5009	0.5862	0.127*	0.509 (13)
C54A	0.6329 (4)	0.4375 (4)	0.4781 (5)	0.066 (4)*	0.509 (13)

H54A	0.6385	0.4032	0.5114	0.099*	0.509 (13)
H54B	0.6460	0.4192	0.4461	0.099*	0.509 (13)
H54C	0.5955	0.4473	0.4599	0.099*	0.509 (13)
C55A	0.7203 (3)	0.4892 (7)	0.5317 (5)	0.065 (3)*	0.509 (13)
H55A	0.7402	0.5315	0.5475	0.098*	0.509 (13)
H55B	0.7318	0.4692	0.4990	0.098*	0.509 (13)
H55C	0.7262	0.4558	0.5656	0.098*	0.509 (13)
C53C	0.6731 (5)	0.5583 (5)	0.5615 (4)	0.076 (4)*	0.491 (13)
H53D	0.6421	0.5874	0.5552	0.114*	0.491 (13)
H53E	0.7031	0.5877	0.5640	0.114*	0.491 (13)
H53F	0.6802	0.5322	0.6002	0.114*	0.491 (13)
C54C	0.6181 (4)	0.4632 (7)	0.5069 (7)	0.094 (5)*	0.491 (13)
H54D	0.6295	0.4310	0.5420	0.142*	0.491 (13)
H54E	0.6048	0.4369	0.4681	0.142*	0.491 (13)
H54F	0.5904	0.4931	0.5114	0.142*	0.491 (13)
C55C	0.7122 (4)	0.4651 (6)	0.5162 (5)	0.058 (3)*	0.491 (13)
H55D	0.7409	0.4965	0.5174	0.086*	0.491 (13)
H55E	0.7070	0.4317	0.4825	0.086*	0.491 (13)
H55F	0.7207	0.4404	0.5558	0.086*	0.491 (13)
C56	0.63724 (19)	0.5851 (2)	0.27216 (19)	0.0427 (11)	
C57	0.6336 (2)	0.5622 (2)	0.2068 (2)	0.0522 (12)	
C58	0.6867 (2)	0.5642 (4)	0.1979 (3)	0.0837 (19)	
H58A	0.7009	0.6112	0.2057	0.126*	
H58B	0.6829	0.5506	0.1553	0.126*	
H58C	0.7104	0.5320	0.2270	0.126*	
C59	0.5964 (2)	0.6136 (3)	0.1631 (2)	0.0734 (16)	
H59A	0.5926	0.6018	0.1200	0.110*	
H59B	0.6106	0.6605	0.1723	0.110*	
H59C	0.5623	0.6114	0.1689	0.110*	
C60	0.6108 (2)	0.4889 (3)	0.1945 (2)	0.0713 (16)	
H60A	0.6076	0.4749	0.1522	0.107*	
H60B	0.5763	0.4883	0.1994	0.107*	
H60C	0.6340	0.4566	0.2242	0.107*	
C61	0.49427 (19)	0.5246 (2)	0.2712 (2)	0.0499 (11)	
H61	0.5054	0.5451	0.2399	0.060*	
C62	0.4604 (2)	0.4690 (2)	0.2555 (2)	0.0592 (13)	
H62	0.4490	0.4513	0.2144	0.071*	
C63	0.4436 (2)	0.4399 (3)	0.3000 (3)	0.0636 (14)	
H63	0.4205	0.4016	0.2903	0.076*	
C64	0.4606 (2)	0.4668 (3)	0.3589 (2)	0.0612 (14)	
H64	0.4489	0.4476	0.3903	0.073*	
C65	0.49491 (19)	0.5220 (2)	0.3722 (2)	0.0536 (12)	
H65	0.5067	0.5401	0.4131	0.064*	
C66	0.50690 (17)	0.7380 (2)	0.26840 (19)	0.0435 (10)	
C67	0.45471 (19)	0.7499 (2)	0.2182 (2)	0.0597 (13)	
C68A	0.4480 (5)	0.6963 (5)	0.1655 (4)	0.096 (4)*	0.595 (10)
H68A	0.4170	0.7080	0.1302	0.144*	0.595 (10)
H68B	0.4438	0.6499	0.1807	0.144*	0.595 (10)

H68C	0.4789	0.6970	0.1524	0.144*	0.595 (10)
C69A	0.4127 (4)	0.7418 (7)	0.2461 (6)	0.112 (5)*	0.595 (10)
H69A	0.3787	0.7415	0.2132	0.167*	0.595 (10)
H69B	0.4142	0.7805	0.2744	0.167*	0.595 (10)
H69C	0.4176	0.6981	0.2692	0.167*	0.595 (10)
C70A	0.4529 (4)	0.8195 (4)	0.1866 (4)	0.067 (3)*	0.595 (10)
H70A	0.4828	0.8235	0.1718	0.100*	0.595 (10)
H70B	0.4543	0.8567	0.2163	0.100*	0.595 (10)
H70C	0.4204	0.8232	0.1514	0.100*	0.595 (10)
C68C	0.4642 (7)	0.7556 (10)	0.1581 (5)	0.116 (7)*	0.405 (10)
H68D	0.4931	0.7877	0.1624	0.173*	0.405 (10)
H68E	0.4327	0.7728	0.1263	0.173*	0.405 (10)
H68F	0.4732	0.7099	0.1458	0.173*	0.405 (10)
C69C	0.4156 (5)	0.6958 (7)	0.2215 (7)	0.079 (5)*	0.405 (10)
H69D	0.4253	0.6509	0.2086	0.119*	0.405 (10)
H69E	0.3808	0.7089	0.1939	0.119*	0.405 (10)
H69F	0.4154	0.6925	0.2642	0.119*	0.405 (10)
C70C	0.4340 (7)	0.8191 (7)	0.2353 (9)	0.137 (9)*	0.405 (10)
H70D	0.4624	0.8531	0.2474	0.205*	0.405 (10)
H70E	0.4209	0.8114	0.2699	0.205*	0.405 (10)
H70F	0.4057	0.8364	0.1990	0.205*	0.405 (10)
C71	0.53819 (17)	0.7238 (2)	0.44541 (19)	0.0400 (10)	
C72	0.51769 (18)	0.7226 (2)	0.49973 (19)	0.0451 (11)	
C73	0.4863 (2)	0.6575 (3)	0.4989 (2)	0.0640 (14)	
H73A	0.4741	0.6575	0.5347	0.096*	
H73B	0.5083	0.6168	0.5008	0.096*	
H73C	0.4562	0.6561	0.4606	0.096*	
C74	0.4831 (2)	0.7862 (3)	0.4956 (3)	0.0687 (15)	
H74A	0.5038	0.8283	0.4982	0.103*	
H74B	0.4690	0.7854	0.5300	0.103*	
H74C	0.4542	0.7856	0.4561	0.103*	
C75	0.5641 (2)	0.7256 (3)	0.5602 (2)	0.0658 (14)	
H75A	0.5838	0.7684	0.5613	0.099*	
H75B	0.5868	0.6856	0.5625	0.099*	
H75C	0.5513	0.7247	0.5956	0.099*	
C76	0.59057 (19)	0.9343 (2)	0.4413 (2)	0.0525 (12)	
C77	0.5996 (2)	1.0107 (2)	0.4544 (2)	0.0635 (15)	
C78A	0.5444 (3)	1.0430 (4)	0.4226 (4)	0.067 (3)*	0.677 (11)
H78A	0.5195	1.0224	0.4404	0.100*	0.677 (11)
H78B	0.5329	1.0336	0.3779	0.100*	0.677 (11)
H78C	0.5460	1.0931	0.4296	0.100*	0.677 (11)
C79A	0.6138 (4)	1.0278 (5)	0.5210 (4)	0.076 (3)*	0.677 (11)
H79A	0.6216	1.0773	0.5270	0.114*	0.677 (11)
H79B	0.6446	1.0010	0.5446	0.114*	0.677 (11)
H79C	0.5846	1.0163	0.5355	0.114*	0.677 (11)
C80A	0.6358 (3)	1.0365 (4)	0.4223 (4)	0.065 (2)*	0.677 (11)
H80A	0.6207	1.0273	0.3777	0.097*	0.677 (11)
H80B	0.6694	1.0128	0.4390	0.097*	0.677 (11)

H80C	0.6410	1.0865	0.4292	0.097*	0.677 (11)
C78C	0.5553 (8)	1.0427 (10)	0.4699 (14)	0.176 (15)*	0.323 (11)
H78D	0.5633	1.0913	0.4813	0.264*	0.323 (11)
H78E	0.5501	1.0178	0.5049	0.264*	0.323 (11)
H78F	0.5234	1.0399	0.4338	0.264*	0.323 (11)
C79C	0.6484 (7)	1.0168 (10)	0.5138 (7)	0.096 (7)*	0.323 (11)
H79D	0.6522	1.0649	0.5285	0.144*	0.323 (11)
H79E	0.6796	1.0030	0.5042	0.144*	0.323 (11)
H79F	0.6441	0.9865	0.5462	0.144*	0.323 (11)
C80C	0.6120 (9)	1.0470 (9)	0.4029 (7)	0.092 (7)*	0.323 (11)
H80D	0.5817	1.0448	0.3649	0.138*	0.323 (11)
H80E	0.6419	1.0245	0.3958	0.138*	0.323 (11)
H80F	0.6206	1.0955	0.4143	0.138*	0.323 (11)
C81	0.70860 (18)	0.7746 (2)	0.4815 (2)	0.0483 (11)	
C82	0.74610 (19)	0.7975 (3)	0.5435 (2)	0.0650 (14)	
C83A	0.7488 (6)	0.7459 (6)	0.5931 (5)	0.112 (5)*	0.526 (12)
H83A	0.7662	0.7038	0.5860	0.167*	0.526 (12)
H83B	0.7134	0.7345	0.5922	0.167*	0.526 (12)
H83C	0.7686	0.7655	0.6337	0.167*	0.526 (12)
C84A	0.7988 (3)	0.8095 (7)	0.5352 (6)	0.085 (4)*	0.526 (12)
H84A	0.8234	0.8280	0.5738	0.127*	0.526 (12)
H84B	0.7948	0.8427	0.5015	0.127*	0.526 (12)
H84C	0.8121	0.7656	0.5251	0.127*	0.526 (12)
C85A	0.7283 (5)	0.8683 (5)	0.5603 (6)	0.100 (5)*	0.526 (12)
H85A	0.7513	0.8824	0.6015	0.149*	0.526 (12)
H85B	0.6924	0.8648	0.5604	0.149*	0.526 (12)
H85C	0.7301	0.9028	0.5295	0.149*	0.526 (12)
C83C	0.7805 (5)	0.7368 (6)	0.5784 (6)	0.097 (5)*	0.474 (12)
H83D	0.8035	0.7219	0.5556	0.146*	0.474 (12)
H83E	0.7582	0.6981	0.5815	0.146*	0.474 (12)
H83F	0.8016	0.7520	0.6201	0.146*	0.474 (12)
C84C	0.7805 (6)	0.8536 (8)	0.5325 (7)	0.124 (7)*	0.474 (12)
H84D	0.7920	0.8405	0.4977	0.185*	0.474 (12)
H84E	0.8110	0.8597	0.5699	0.185*	0.474 (12)
H84F	0.7609	0.8971	0.5228	0.185*	0.474 (12)
C85C	0.7156 (5)	0.8194 (8)	0.5847 (6)	0.106 (6)*	0.474 (12)
H85D	0.7398	0.8325	0.6256	0.159*	0.474 (12)
H85E	0.6937	0.7809	0.5893	0.159*	0.474 (12)
H85F	0.6935	0.8591	0.5661	0.159*	0.474 (12)
C86	0.68681 (19)	0.8154 (2)	0.31200 (19)	0.0472 (11)	
C87	0.71799 (19)	0.8586 (2)	0.2812 (2)	0.0622 (14)	
C88A	0.6977 (5)	0.8357 (6)	0.2126 (4)	0.089 (4)*	0.586 (14)
H88A	0.7129	0.8655	0.1882	0.134*	0.586 (14)
H88B	0.6596	0.8396	0.1966	0.134*	0.586 (14)
H88C	0.7079	0.7876	0.2093	0.134*	0.586 (14)
C89A	0.7748 (3)	0.8427 (8)	0.3070 (7)	0.111 (5)*	0.586 (14)
H89A	0.7815	0.7975	0.2918	0.166*	0.586 (14)
H89B	0.7858	0.8419	0.3524	0.166*	0.586 (14)

H89C	0.7945	0.8784	0.2937	0.166*	0.586 (14)
C90A	0.7050 (4)	0.9347 (4)	0.2841 (4)	0.076 (3)*	0.586 (14)
H90A	0.7211	0.9517	0.3267	0.114*	0.586 (14)
H90B	0.6671	0.9405	0.2715	0.114*	0.586 (14)
H90C	0.7185	0.9612	0.2561	0.114*	0.586 (14)
C88C	0.7318 (8)	0.8176 (4)	0.2333 (5)	0.116 (7)*	0.414 (14)
H88D	0.7406	0.8492	0.2047	0.174*	0.414 (14)
H88E	0.7020	0.7888	0.2101	0.174*	0.414 (14)
H88F	0.7619	0.7879	0.2537	0.174*	0.414 (14)
C89C	0.7707 (4)	0.8731 (8)	0.3326 (6)	0.074 (5)*	0.414 (14)
H89D	0.7898	0.8296	0.3452	0.112*	0.414 (14)
H89E	0.7642	0.8941	0.3684	0.112*	0.414 (14)
H89F	0.7914	0.9049	0.3167	0.112*	0.414 (14)
C90C	0.6928 (6)	0.9260 (6)	0.2546 (8)	0.085 (5)*	0.414 (14)
H90D	0.6805	0.9496	0.2851	0.128*	0.414 (14)
H90E	0.6631	0.9169	0.2169	0.128*	0.414 (14)
H90F	0.7183	0.9553	0.2444	0.128*	0.414 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1A	0.0437 (4)	0.0415 (3)	0.0327 (3)	0.0003 (3)	0.0133 (3)	−0.0034 (3)
Mn2A	0.0494 (4)	0.0452 (4)	0.0317 (3)	0.0020 (3)	0.0163 (3)	−0.0004 (3)
Mn3A	0.0498 (4)	0.0578 (4)	0.0356 (4)	0.0080 (3)	0.0145 (3)	0.0020 (3)
O1	0.0468 (18)	0.0433 (16)	0.0340 (15)	0.0017 (13)	0.0160 (13)	−0.0012 (12)
O2	0.071 (2)	0.0449 (17)	0.0441 (18)	0.0051 (16)	0.0211 (17)	0.0001 (14)
O3	0.063 (2)	0.0521 (19)	0.0427 (17)	−0.0023 (16)	0.0237 (15)	−0.0010 (14)
O4	0.057 (2)	0.0578 (19)	0.0378 (17)	0.0017 (16)	0.0157 (15)	−0.0055 (14)
O5	0.0505 (19)	0.0564 (19)	0.0426 (18)	−0.0019 (15)	0.0169 (14)	−0.0115 (14)
O6	0.054 (2)	0.074 (2)	0.0410 (18)	0.0046 (17)	0.0187 (16)	0.0013 (15)
O7	0.049 (2)	0.094 (3)	0.0416 (19)	0.0028 (18)	0.0146 (15)	0.0020 (17)
O8	0.061 (2)	0.0528 (18)	0.0399 (17)	0.0035 (16)	0.0203 (15)	−0.0018 (14)
O9	0.069 (2)	0.056 (2)	0.049 (2)	0.0113 (17)	0.0142 (17)	0.0014 (16)
O10	0.060 (3)	0.087 (3)	0.061 (2)	0.009 (2)	0.0108 (19)	0.002 (2)
O11	0.070 (3)	0.185 (5)	0.080 (3)	0.005 (3)	0.014 (2)	0.027 (3)
O12	0.064 (2)	0.061 (2)	0.060 (2)	0.0128 (18)	0.0292 (17)	0.0146 (16)
O13	0.058 (2)	0.0451 (18)	0.0477 (18)	−0.0009 (15)	0.0264 (15)	−0.0017 (14)
O14	0.051 (2)	0.064 (2)	0.0421 (18)	0.0025 (16)	0.0111 (15)	−0.0029 (15)
O15	0.0478 (19)	0.0561 (19)	0.0388 (16)	−0.0036 (14)	0.0164 (14)	−0.0030 (13)
N1	0.049 (2)	0.047 (2)	0.038 (2)	0.0018 (17)	0.0102 (17)	−0.0051 (16)
N2	0.054 (2)	0.055 (2)	0.037 (2)	0.0007 (19)	0.0202 (18)	−0.0011 (17)
C1	0.057 (3)	0.059 (3)	0.063 (3)	0.003 (3)	0.028 (3)	−0.012 (2)
C2	0.070 (4)	0.082 (4)	0.077 (4)	0.015 (3)	0.041 (3)	−0.009 (3)
C3	0.085 (4)	0.074 (4)	0.060 (3)	0.030 (3)	0.031 (3)	−0.002 (3)
C4	0.098 (5)	0.050 (3)	0.059 (3)	0.019 (3)	0.020 (3)	−0.007 (2)
C5	0.070 (3)	0.044 (3)	0.046 (3)	0.002 (2)	0.012 (2)	−0.002 (2)
C6	0.065 (3)	0.050 (3)	0.039 (3)	−0.008 (2)	0.011 (2)	−0.004 (2)
C7	0.134 (6)	0.047 (3)	0.060 (3)	0.000 (3)	0.042 (4)	0.004 (2)

C11	0.054 (3)	0.042 (2)	0.046 (3)	−0.002 (2)	0.016 (2)	−0.010 (2)
C12	0.044 (3)	0.077 (3)	0.053 (3)	0.003 (2)	0.008 (2)	−0.019 (3)
C13	0.064 (4)	0.130 (6)	0.082 (4)	−0.029 (4)	0.017 (3)	−0.020 (4)
C14	0.066 (4)	0.107 (5)	0.091 (5)	0.033 (4)	−0.005 (3)	−0.027 (4)
C15	0.067 (4)	0.119 (5)	0.051 (3)	0.009 (4)	−0.003 (3)	−0.016 (3)
C16	0.059 (3)	0.061 (3)	0.042 (3)	0.000 (2)	0.022 (2)	0.002 (2)
C17	0.071 (4)	0.081 (4)	0.044 (3)	0.004 (3)	0.028 (3)	0.007 (3)
C18	0.073 (4)	0.089 (4)	0.037 (3)	0.007 (3)	0.019 (3)	0.000 (3)
C19	0.065 (4)	0.079 (4)	0.036 (3)	0.004 (3)	0.013 (2)	−0.008 (2)
C20	0.058 (3)	0.059 (3)	0.047 (3)	−0.002 (2)	0.021 (2)	−0.008 (2)
C21	0.048 (3)	0.065 (3)	0.050 (3)	0.006 (2)	0.023 (2)	0.004 (2)
C22	0.056 (3)	0.114 (5)	0.072 (4)	0.022 (3)	0.035 (3)	0.029 (3)
C26	0.054 (3)	0.052 (3)	0.050 (3)	0.005 (2)	0.030 (2)	0.000 (2)
C27	0.097 (4)	0.048 (3)	0.061 (3)	0.008 (3)	0.030 (3)	0.005 (2)
C31	0.076 (5)	0.098 (5)	0.066 (4)	0.013 (4)	0.025 (4)	0.011 (3)
C32	0.079 (4)	0.109 (5)	0.073 (4)	0.021 (4)	0.009 (3)	0.007 (4)
C36	0.060 (3)	0.054 (3)	0.039 (2)	0.002 (2)	0.021 (2)	−0.001 (2)
C37	0.066 (3)	0.055 (3)	0.061 (3)	−0.004 (3)	0.032 (3)	0.003 (2)
C38	0.101 (5)	0.060 (3)	0.089 (4)	−0.001 (3)	0.047 (4)	0.017 (3)
C39	0.074 (4)	0.067 (4)	0.082 (4)	−0.023 (3)	0.026 (3)	−0.006 (3)
C40	0.084 (4)	0.072 (4)	0.077 (4)	−0.009 (3)	0.052 (3)	−0.002 (3)
C41	0.050 (3)	0.064 (3)	0.044 (3)	−0.007 (2)	0.018 (2)	−0.007 (2)
C42	0.056 (4)	0.072 (4)	0.103 (5)	−0.012 (3)	−0.005 (3)	−0.008 (3)
Mn1B	0.0428 (4)	0.0396 (3)	0.0412 (4)	−0.0007 (3)	0.0151 (3)	−0.0010 (3)
Mn2B	0.0434 (4)	0.0350 (3)	0.0310 (3)	−0.0008 (3)	0.0115 (3)	−0.0001 (3)
Mn3B	0.0513 (4)	0.0346 (3)	0.0378 (3)	−0.0005 (3)	0.0159 (3)	−0.0011 (3)
O16	0.0424 (17)	0.0374 (15)	0.0376 (15)	−0.0019 (12)	0.0146 (13)	−0.0011 (12)
O17	0.051 (2)	0.0442 (17)	0.0446 (17)	0.0074 (14)	0.0164 (15)	0.0051 (13)
O18	0.0446 (19)	0.0455 (17)	0.0384 (16)	−0.0010 (14)	0.0123 (14)	0.0039 (13)
O19	0.0541 (19)	0.0483 (17)	0.0434 (17)	−0.0023 (15)	0.0241 (15)	−0.0018 (14)
O20	0.0532 (19)	0.0429 (17)	0.0422 (17)	−0.0057 (14)	0.0236 (15)	−0.0052 (13)
O21	0.0504 (18)	0.0433 (17)	0.0371 (16)	0.0013 (14)	0.0108 (13)	0.0008 (13)
O22	0.055 (2)	0.0407 (17)	0.0512 (18)	0.0067 (15)	0.0130 (15)	0.0002 (14)
O23	0.0481 (18)	0.0447 (17)	0.0397 (16)	−0.0039 (14)	0.0166 (13)	−0.0054 (14)
O24	0.071 (2)	0.0412 (17)	0.0489 (18)	−0.0068 (15)	0.0301 (16)	−0.0082 (14)
O25	0.075 (2)	0.0425 (17)	0.0366 (17)	0.0059 (15)	0.0168 (15)	−0.0018 (14)
O26	0.097 (3)	0.0452 (18)	0.0489 (19)	−0.0059 (18)	0.0350 (19)	−0.0065 (15)
O27	0.058 (2)	0.0443 (18)	0.0488 (18)	−0.0027 (15)	0.0133 (16)	−0.0084 (14)
O28	0.0480 (19)	0.0516 (19)	0.0448 (17)	0.0016 (15)	0.0099 (14)	−0.0022 (14)
O29	0.057 (2)	0.0516 (19)	0.0506 (19)	0.0017 (16)	0.0219 (16)	0.0081 (15)
O30	0.059 (2)	0.0455 (18)	0.060 (2)	−0.0035 (15)	0.0269 (16)	0.0036 (15)
N3	0.046 (2)	0.051 (2)	0.064 (3)	−0.0022 (18)	0.023 (2)	−0.0042 (19)
N4	0.050 (2)	0.0418 (19)	0.0341 (19)	−0.0006 (17)	0.0115 (16)	−0.0001 (15)
C46	0.051 (3)	0.071 (3)	0.064 (3)	0.002 (3)	0.012 (3)	−0.007 (3)
C47	0.047 (4)	0.110 (5)	0.098 (5)	0.017 (3)	0.003 (3)	−0.015 (4)
C48	0.047 (4)	0.122 (6)	0.136 (7)	−0.001 (4)	0.035 (4)	−0.021 (5)
C49	0.063 (4)	0.087 (4)	0.127 (6)	−0.008 (3)	0.053 (4)	−0.006 (4)
C50	0.058 (4)	0.062 (3)	0.087 (4)	−0.005 (3)	0.036 (3)	0.000 (3)

C51	0.054 (3)	0.038 (2)	0.037 (2)	0.003 (2)	0.018 (2)	−0.0010 (18)
C52	0.057 (3)	0.065 (3)	0.054 (3)	0.015 (2)	0.021 (2)	0.022 (2)
C56	0.058 (3)	0.033 (2)	0.039 (2)	0.009 (2)	0.017 (2)	0.0024 (18)
C57	0.067 (3)	0.058 (3)	0.036 (2)	0.002 (2)	0.022 (2)	−0.002 (2)
C58	0.080 (4)	0.134 (6)	0.050 (3)	0.003 (4)	0.038 (3)	−0.011 (3)
C59	0.102 (5)	0.068 (3)	0.043 (3)	0.010 (3)	0.015 (3)	0.007 (2)
C60	0.106 (5)	0.061 (3)	0.050 (3)	−0.001 (3)	0.031 (3)	−0.012 (2)
C61	0.060 (3)	0.049 (3)	0.038 (2)	−0.003 (2)	0.014 (2)	−0.004 (2)
C62	0.067 (3)	0.052 (3)	0.051 (3)	−0.010 (3)	0.010 (3)	−0.011 (2)
C63	0.066 (4)	0.050 (3)	0.070 (4)	−0.017 (3)	0.016 (3)	−0.005 (3)
C64	0.064 (3)	0.059 (3)	0.065 (3)	−0.019 (3)	0.027 (3)	0.000 (3)
C65	0.063 (3)	0.058 (3)	0.041 (3)	−0.008 (2)	0.019 (2)	0.001 (2)
C66	0.050 (3)	0.042 (3)	0.042 (2)	−0.001 (2)	0.020 (2)	0.001 (2)
C67	0.050 (3)	0.054 (3)	0.066 (3)	0.003 (2)	0.007 (2)	0.005 (2)
C71	0.046 (3)	0.035 (2)	0.038 (2)	0.0022 (19)	0.0131 (19)	0.0003 (18)
C72	0.056 (3)	0.044 (2)	0.040 (2)	−0.001 (2)	0.022 (2)	−0.0024 (19)
C73	0.088 (4)	0.066 (3)	0.050 (3)	−0.020 (3)	0.039 (3)	−0.008 (2)
C74	0.069 (4)	0.067 (3)	0.086 (4)	0.009 (3)	0.047 (3)	−0.001 (3)
C75	0.080 (4)	0.072 (3)	0.045 (3)	−0.009 (3)	0.020 (3)	−0.004 (2)
C76	0.067 (3)	0.046 (3)	0.045 (3)	0.003 (2)	0.019 (2)	−0.001 (2)
C77	0.098 (4)	0.047 (3)	0.043 (3)	−0.004 (3)	0.020 (3)	−0.006 (2)
C81	0.047 (3)	0.054 (3)	0.044 (3)	−0.007 (2)	0.015 (2)	−0.006 (2)
C82	0.059 (3)	0.078 (4)	0.053 (3)	0.000 (3)	0.012 (2)	−0.014 (3)
C86	0.056 (3)	0.044 (3)	0.041 (2)	−0.010 (2)	0.014 (2)	0.000 (2)
C87	0.066 (4)	0.062 (3)	0.066 (3)	0.000 (3)	0.031 (3)	0.019 (3)

Geometric parameters (Å, º)

Mn1A—O1	1.810 (3)	Mn1B—O16	1.818 (3)
Mn1A—O2	2.140 (3)	Mn1B—O17	2.198 (3)
Mn1A—O5	2.004 (3)	Mn1B—O19	1.967 (3)
Mn1A—O13	2.076 (3)	Mn1B—O28	1.962 (3)
Mn1A—O15	2.008 (3)	Mn1B—O30	2.119 (3)
Mn1A—N1	2.084 (4)	Mn1B—N3	2.094 (4)
Mn1A—Mn2A	3.1743 (9)	Mn1B—Mn2B	3.2171 (9)
Mn2A—O1	1.814 (3)	Mn2B—O16	1.816 (3)
Mn2A—O3	1.978 (3)	Mn2B—O18	1.966 (3)
Mn2A—O4	2.167 (3)	Mn2B—O20	2.162 (3)
Mn2A—O6	2.145 (3)	Mn2B—O21	1.960 (3)
Mn2A—O8	1.960 (3)	Mn2B—O23	2.174 (3)
Mn2A—N2	2.081 (3)	Mn2B—N4	2.089 (4)
Mn3A—O1	2.124 (3)	Mn3B—O16	2.109 (3)
Mn3A—O7	2.207 (3)	Mn3B—O22	2.133 (3)
Mn3A—O9	2.130 (3)	Mn3B—O24	2.221 (3)
Mn3A—O10	2.224 (4)	Mn3B—O25	2.251 (3)
Mn3A—O12	2.129 (4)	Mn3B—O27	2.177 (3)
Mn3A—O14	2.169 (3)	Mn3B—O29	2.131 (3)
O2—C6	1.251 (6)	O17—C51	1.246 (5)

O3—C6	1.282 (6)	O18—C51	1.277 (5)
O4—C11	1.247 (5)	O19—C56	1.276 (5)
O5—C11	1.280 (5)	O20—C56	1.246 (5)
O6—C21	1.247 (5)	O21—C66	1.276 (5)
O7—C21	1.271 (5)	O22—C66	1.244 (5)
O8—C26	1.286 (5)	O23—C71	1.249 (5)
O9—C26	1.244 (5)	O24—C71	1.269 (5)
O10—C31	1.198 (7)	O25—C76	1.222 (5)
O11—C31	1.315 (7)	O26—C76	1.320 (5)
O11—H11	0.8400	O26—H26	0.8400
O12—C36	1.247 (6)	O27—C81	1.239 (5)
O13—C36	1.272 (5)	O28—C81	1.282 (5)
O14—C41	1.249 (6)	O29—C86	1.255 (5)
O15—C41	1.282 (5)	O30—C86	1.269 (5)
N1—C5	1.329 (6)	N3—C50	1.329 (7)
N1—C1	1.333 (6)	N3—C46	1.343 (6)
N2—C16	1.339 (6)	N4—C65	1.341 (6)
N2—C20	1.347 (6)	N4—C61	1.348 (5)
C1—C2	1.378 (7)	C46—C47	1.371 (8)
C1—H1	0.9500	C46—H46	0.9500
C2—C3	1.358 (8)	C47—C48	1.393 (10)
C2—H2	0.9500	C47—H47	0.9500
C3—C4	1.365 (8)	C48—C49	1.360 (10)
C3—H3	0.9500	C48—H48	0.9500
C4—C5	1.380 (7)	C49—C50	1.380 (8)
C4—H4	0.9500	C49—H49	0.9500
C5—H5	0.9500	C50—H50	0.9500
C6—C7	1.518 (6)	C51—C52	1.522 (6)
C7—C9C	1.457 (8)	C52—C53A	1.473 (8)
C7—C10A	1.465 (8)	C52—C54C	1.485 (8)
C7—C8A	1.498 (8)	C52—C55C	1.506 (7)
C7—C8C	1.526 (8)	C52—C55A	1.510 (7)
C7—C10C	1.588 (8)	C52—C53C	1.575 (8)
C7—C9A	1.610 (8)	C52—C54A	1.579 (7)
C8A—H8A	0.9800	C53A—H53A	0.9800
C8A—H8B	0.9800	C53A—H53B	0.9800
C8A—H8C	0.9800	C53A—H53C	0.9800
C9A—H9A	0.9800	C54A—H54A	0.9800
C9A—H9B	0.9800	C54A—H54B	0.9800
C9A—H9C	0.9800	C54A—H54C	0.9800
C10A—H10A	0.9800	C55A—H55A	0.9800
C10A—H10B	0.9800	C55A—H55B	0.9800
C10A—H10C	0.9800	C55A—H55C	0.9800
C8C—H8D	0.9800	C53C—H53D	0.9800
C8C—H8E	0.9800	C53C—H53E	0.9800
C8C—H8F	0.9800	C53C—H53F	0.9800
C9C—H9D	0.9800	C54C—H54D	0.9800
C9C—H9E	0.9800	C54C—H54E	0.9800

C9C—H9F	0.9800	C54C—H54F	0.9800
C10C—H10D	0.9800	C55C—H55D	0.9800
C10C—H10E	0.9800	C55C—H55E	0.9800
C10C—H10F	0.9800	C55C—H55F	0.9800
C11—C12	1.522 (7)	C56—C57	1.529 (6)
C12—C13	1.511 (8)	C57—C58	1.523 (7)
C12—C15	1.522 (7)	C57—C59	1.527 (7)
C12—C14	1.536 (7)	C57—C60	1.533 (7)
C13—H13A	0.9800	C58—H58A	0.9800
C13—H13B	0.9800	C58—H58B	0.9800
C13—H13C	0.9800	C58—H58C	0.9800
C14—H14A	0.9800	C59—H59A	0.9800
C14—H14B	0.9800	C59—H59B	0.9800
C14—H14C	0.9800	C59—H59C	0.9800
C15—H15A	0.9800	C60—H60A	0.9800
C15—H15B	0.9800	C60—H60B	0.9800
C15—H15C	0.9800	C60—H60C	0.9800
C16—C17	1.380 (6)	C61—C62	1.381 (6)
C16—H16	0.9500	C61—H61	0.9500
C17—C18	1.371 (7)	C62—C63	1.365 (7)
C17—H17	0.9500	C62—H62	0.9500
C18—C19	1.374 (8)	C63—C64	1.371 (7)
C18—H18	0.9500	C63—H63	0.9500
C19—C20	1.372 (6)	C64—C65	1.382 (7)
C19—H19	0.9500	C64—H64	0.9500
C20—H20	0.9500	C65—H65	0.9500
C21—C22	1.498 (7)	C66—C67	1.517 (6)
C22—C24A	1.471 (7)	C67—C68C	1.483 (8)
C22—C25C	1.485 (8)	C67—C69A	1.489 (8)
C22—C23C	1.490 (8)	C67—C69C	1.509 (8)
C22—C23A	1.499 (7)	C67—C70A	1.518 (7)
C22—C24C	1.606 (9)	C67—C70C	1.550 (9)
C22—C25A	1.608 (8)	C67—C68A	1.551 (7)
C23A—H23A	0.9800	C68A—H68A	0.9800
C23A—H23B	0.9800	C68A—H68B	0.9800
C23A—H23C	0.9800	C68A—H68C	0.9800
C24A—H24A	0.9800	C69A—H69A	0.9800
C24A—H24B	0.9800	C69A—H69B	0.9800
C24A—H24C	0.9800	C69A—H69C	0.9800
C25A—H25A	0.9800	C70A—H70A	0.9800
C25A—H25B	0.9800	C70A—H70B	0.9800
C25A—H25C	0.9800	C70A—H70C	0.9800
C23C—H23D	0.9800	C68C—H68D	0.9800
C23C—H23E	0.9800	C68C—H68E	0.9800
C23C—H23F	0.9800	C68C—H68F	0.9800
C24C—H24D	0.9800	C69C—H69D	0.9800
C24C—H24E	0.9800	C69C—H69E	0.9800
C24C—H24F	0.9800	C69C—H69F	0.9800

C25C—H25D	0.9800	C70C—H70D	0.9800
C25C—H25E	0.9800	C70C—H70E	0.9800
C25C—H25F	0.9800	C70C—H70F	0.9800
C26—C27	1.513 (7)	C71—C72	1.519 (6)
C27—C28A	1.461 (13)	C72—C73	1.516 (6)
C27—C29C	1.504 (9)	C72—C74	1.531 (6)
C27—C30C	1.509 (9)	C72—C75	1.532 (6)
C27—C28C	1.539 (8)	C73—H73A	0.9800
C27—C30A	1.543 (10)	C73—H73B	0.9800
C27—C29A	1.601 (12)	C73—H73C	0.9800
C28A—H28A	0.9800	C74—H74A	0.9800
C28A—H28B	0.9800	C74—H74B	0.9800
C28A—H28C	0.9800	C74—H74C	0.9800
C29A—H29A	0.9800	C75—H75A	0.9800
C29A—H29B	0.9800	C75—H75B	0.9800
C29A—H29C	0.9800	C75—H75C	0.9800
C30A—H30A	0.9800	C76—C77	1.509 (6)
C30A—H30B	0.9800	C77—C79A	1.478 (9)
C30A—H30C	0.9800	C77—C80A	1.493 (7)
C28C—H28D	0.9800	C77—C78C	1.499 (7)
C28C—H28E	0.9800	C77—C80C	1.500 (9)
C28C—H28F	0.9800	C77—C79C	1.556 (9)
C29C—H29D	0.9800	C77—C78A	1.565 (7)
C29C—H29E	0.9800	C78A—H78A	0.9800
C29C—H29F	0.9800	C78A—H78B	0.9800
C30C—H30D	0.9800	C78A—H78C	0.9800
C30C—H30E	0.9800	C79A—H79A	0.9800
C30C—H30F	0.9800	C79A—H79B	0.9800
C31—C32	1.516 (8)	C79A—H79C	0.9800
C32—C35C	1.506 (9)	C80A—H80A	0.9800
C32—C34A	1.510 (10)	C80A—H80B	0.9800
C32—C33C	1.518 (7)	C80A—H80C	0.9800
C32—C35A	1.522 (7)	C78C—H78D	0.9888
C32—C34C	1.522 (9)	C78C—H78E	0.9887
C32—C33A	1.536 (8)	C78C—H78F	0.9890
C33A—H33A	0.9800	C79C—H79D	0.9800
C33A—H33B	0.9800	C79C—H79E	0.9800
C33A—H33C	0.9800	C79C—H79F	0.9800
C34A—H34A	0.9800	C80C—H80D	0.9800
C34A—H34B	0.9800	C80C—H80E	0.9800
C34A—H34C	0.9800	C80C—H80F	0.9800
C35A—H35A	0.9800	C81—C82	1.512 (6)
C35A—H35B	0.9800	C82—C83A	1.493 (8)
C35A—H35C	0.9800	C82—C84C	1.505 (8)
C33C—H33D	0.9800	C82—C85C	1.506 (8)
C33C—H33E	0.9800	C82—C84A	1.523 (8)
C33C—H33F	0.9800	C82—C85A	1.540 (8)
C34C—H34D	0.9847	C82—C83C	1.544 (8)

C34C—H34E	0.9846	C83A—H83A	0.9800
C34C—H34F	0.9847	C83A—H83B	0.9800
C35C—H35D	0.9900	C83A—H83C	0.9800
C35C—H35E	0.9800	C84A—H84A	0.9800
C35C—H35F	0.9800	C84A—H84B	0.9800
C36—C37	1.522 (7)	C84A—H84C	0.9800
C37—C38	1.521 (7)	C85A—H85A	0.9800
C37—C39	1.533 (7)	C85A—H85B	0.9800
C37—C40	1.547 (7)	C85A—H85C	0.9800
C38—H38A	0.9800	C83C—H83D	0.9800
C38—H38B	0.9800	C83C—H83E	0.9800
C38—H38C	0.9800	C83C—H83F	0.9800
C39—H39A	0.9800	C84C—H84D	0.9800
C39—H39B	0.9800	C84C—H84E	0.9800
C39—H39C	0.9800	C84C—H84F	0.9800
C40—H40A	0.9800	C85C—H85D	0.9800
C40—H40B	0.9800	C85C—H85E	0.9800
C40—H40C	0.9800	C85C—H85F	0.9800
C41—C42	1.516 (7)	C86—C87	1.517 (6)
C42—C44C	1.471 (8)	C87—C89A	1.490 (8)
C42—C43A	1.474 (8)	C87—C88C	1.496 (7)
C42—C45A	1.525 (8)	C87—C90C	1.502 (8)
C42—C43C	1.524 (9)	C87—C90A	1.519 (6)
C42—C45C	1.555 (9)	C87—C88A	1.544 (7)
C42—C44A	1.568 (8)	C87—C89C	1.546 (8)
C43A—H43A	0.9800	C88A—H88A	0.9800
C43A—H43B	0.9800	C88A—H88B	0.9800
C43A—H43C	0.9800	C88A—H88C	0.9800
C44A—H44A	0.9800	C89A—H89A	0.9800
C44A—H44B	0.9800	C89A—H89B	0.9800
C44A—H44C	0.9800	C89A—H89C	0.9800
C45A—H45A	0.9800	C90A—H90A	0.9800
C45A—H45B	0.9800	C90A—H90B	0.9800
C45A—H45C	0.9800	C90A—H90C	0.9800
C43C—H43D	0.9800	C88C—H88D	0.9800
C43C—H43E	0.9800	C88C—H88E	0.9799
C43C—H43F	0.9800	C88C—H88F	0.9800
C44C—H44D	0.9800	C89C—H89D	0.9800
C44C—H44E	0.9800	C89C—H89E	0.9800
C44C—H44F	0.9800	C89C—H89F	0.9800
C45C—H45D	0.9800	C90C—H90D	0.9800
C45C—H45E	0.9800	C90C—H90E	0.9800
C45C—H45F	0.9800	C90C—H90F	0.9800

O1—Mn1A—O5	97.22 (12)	O16—Mn1B—O28	96.01 (13)
O1—Mn1A—O15	93.08 (13)	O16—Mn1B—O19	95.17 (12)
O5—Mn1A—O15	167.07 (13)	O28—Mn1B—O19	168.71 (13)
O1—Mn1A—O13	96.19 (12)	O16—Mn1B—N3	178.90 (14)

O5—Mn1A—O13	87.52 (13)	O28—Mn1B—N3	84.62 (14)
O15—Mn1A—O13	99.13 (12)	O19—Mn1B—N3	84.18 (14)
O1—Mn1A—N1	177.67 (13)	O16—Mn1B—O30	97.78 (12)
O5—Mn1A—N1	84.92 (13)	O28—Mn1B—O30	91.71 (13)
O15—Mn1A—N1	84.93 (13)	O19—Mn1B—O30	88.33 (12)
O13—Mn1A—N1	82.96 (13)	N3—Mn1B—O30	83.09 (14)
O1—Mn1A—O2	96.20 (13)	O16—Mn1B—O17	94.07 (12)
O5—Mn1A—O2	87.01 (13)	O28—Mn1B—O17	84.78 (12)
O15—Mn1A—O2	84.13 (12)	O19—Mn1B—O17	92.87 (12)
O13—Mn1A—O2	166.99 (13)	N3—Mn1B—O17	85.09 (14)
N1—Mn1A—O2	84.81 (14)	O30—Mn1B—O17	167.94 (13)
O1—Mn1A—Mn2A	28.86 (8)	O16—Mn1B—Mn2B	27.68 (8)
O5—Mn1A—Mn2A	79.25 (9)	O28—Mn1B—Mn2B	110.04 (10)
O15—Mn1A—Mn2A	106.95 (9)	O19—Mn1B—Mn2B	79.56 (9)
O13—Mn1A—Mn2A	117.51 (9)	N3—Mn1B—Mn2B	151.22 (11)
N1—Mn1A—Mn2A	153.17 (10)	O30—Mn1B—Mn2B	119.70 (9)
O2—Mn1A—Mn2A	72.94 (9)	O17—Mn1B—Mn2B	72.28 (8)
O1—Mn2A—O8	94.26 (12)	O16—Mn2B—O21	95.90 (12)
O1—Mn2A—O3	95.39 (12)	O16—Mn2B—O18	94.97 (12)
O8—Mn2A—O3	170.27 (12)	O21—Mn2B—O18	168.63 (13)
O1—Mn2A—N2	178.47 (15)	O16—Mn2B—N4	176.27 (14)
O8—Mn2A—N2	84.88 (14)	O21—Mn2B—N4	84.85 (13)
O3—Mn2A—N2	85.44 (13)	O18—Mn2B—N4	84.52 (12)
O1—Mn2A—O6	96.73 (12)	O16—Mn2B—O20	92.46 (12)
O8—Mn2A—O6	92.40 (13)	O21—Mn2B—O20	89.72 (12)
O3—Mn2A—O6	87.68 (13)	O18—Mn2B—O20	93.16 (12)
N2—Mn2A—O6	84.58 (13)	N4—Mn2B—O20	83.88 (13)
O1—Mn2A—O4	96.51 (12)	O16—Mn2B—O23	96.62 (12)
O8—Mn2A—O4	89.39 (13)	O21—Mn2B—O23	90.67 (12)
O3—Mn2A—O4	88.31 (13)	O18—Mn2B—O23	84.76 (12)
N2—Mn2A—O4	82.23 (13)	N4—Mn2B—O23	87.02 (13)
O6—Mn2A—O4	166.47 (12)	O20—Mn2B—O23	170.82 (11)
O1—Mn2A—Mn1A	28.79 (9)	O16—Mn2B—Mn1B	27.71 (9)
O8—Mn2A—Mn1A	109.80 (9)	O21—Mn2B—Mn1B	112.65 (9)
O3—Mn2A—Mn1A	78.52 (9)	O18—Mn2B—Mn1B	78.66 (9)
N2—Mn2A—Mn1A	150.64 (11)	N4—Mn2B—Mn1B	148.95 (10)
O6—Mn2A—Mn1A	118.76 (9)	O20—Mn2B—Mn1B	71.32 (8)
O4—Mn2A—Mn1A	72.95 (8)	O23—Mn2B—Mn1B	116.83 (8)
O1—Mn3A—O12	93.75 (12)	O16—Mn3B—O29	98.38 (12)
O1—Mn3A—O9	90.95 (11)	O16—Mn3B—O22	93.07 (11)
O12—Mn3A—O9	89.61 (14)	O29—Mn3B—O22	92.58 (12)
O1—Mn3A—O14	89.54 (11)	O16—Mn3B—O27	91.68 (11)
O12—Mn3A—O14	99.21 (13)	O29—Mn3B—O27	91.55 (12)
O9—Mn3A—O14	171.12 (14)	O22—Mn3B—O27	173.19 (12)
O1—Mn3A—O7	95.15 (12)	O16—Mn3B—O24	90.08 (11)
O12—Mn3A—O7	170.04 (13)	O29—Mn3B—O24	170.89 (12)
O9—Mn3A—O7	85.80 (14)	O22—Mn3B—O24	90.30 (12)
O14—Mn3A—O7	85.32 (13)	O27—Mn3B—O24	84.82 (12)

O1—Mn3A—O10	172.46 (13)	O16—Mn3B—O25	170.09 (11)
O12—Mn3A—O10	85.81 (14)	O29—Mn3B—O25	89.31 (12)
O9—Mn3A—O10	96.57 (13)	O22—Mn3B—O25	92.81 (11)
O14—Mn3A—O10	83.11 (13)	O27—Mn3B—O25	81.82 (11)
O7—Mn3A—O10	85.94 (14)	O24—Mn3B—O25	81.92 (11)
Mn1A—O1—Mn2A	122.36 (15)	Mn1B—O16—Mn2B	124.60 (15)
Mn1A—O1—Mn3A	118.09 (14)	Mn1B—O16—Mn3B	115.50 (13)
Mn2A—O1—Mn3A	119.55 (14)	Mn2B—O16—Mn3B	119.88 (14)
C6—O2—Mn1A	128.5 (3)	C51—O17—Mn1B	126.9 (3)
C6—O3—Mn2A	128.3 (3)	C51—O18—Mn2B	130.6 (3)
C11—O4—Mn2A	130.0 (3)	C56—O19—Mn1B	128.7 (3)
C11—O5—Mn1A	126.2 (3)	C56—O20—Mn2B	128.3 (3)
C21—O6—Mn2A	139.2 (3)	C66—O21—Mn2B	132.1 (3)
C21—O7—Mn3A	126.2 (3)	C66—O22—Mn3B	132.4 (3)
C26—O8—Mn2A	131.6 (3)	C71—O23—Mn2B	133.0 (3)
C26—O9—Mn3A	131.8 (3)	C71—O24—Mn3B	129.6 (3)
C31—O10—Mn3A	129.1 (4)	C76—O25—Mn3B	129.4 (3)
C31—O11—H11	109.5	C76—O26—H26	109.5
C36—O12—Mn3A	127.4 (3)	C81—O27—Mn3B	132.2 (3)
C36—O13—Mn1A	135.3 (3)	C81—O28—Mn1B	129.8 (3)
C41—O14—Mn3A	128.2 (3)	C86—O29—Mn3B	122.7 (3)
C41—O15—Mn1A	130.8 (3)	C86—O30—Mn1B	139.4 (3)
C5—N1—C1	117.8 (4)	C50—N3—C46	118.3 (5)
C5—N1—Mn1A	121.9 (3)	C50—N3—Mn1B	119.8 (4)
C1—N1—Mn1A	120.2 (3)	C46—N3—Mn1B	121.9 (4)
C16—N2—C20	118.4 (4)	C65—N4—C61	117.8 (4)
C16—N2—Mn2A	121.4 (3)	C65—N4—Mn2B	122.1 (3)
C20—N2—Mn2A	120.2 (3)	C61—N4—Mn2B	120.0 (3)
N1—C1—C2	122.1 (5)	N3—C46—C47	122.5 (6)
N1—C1—H1	118.9	N3—C46—H46	118.7
C2—C1—H1	118.9	C47—C46—H46	118.7
C3—C2—C1	120.0 (6)	C46—C47—C48	118.8 (6)
C3—C2—H2	120.0	C46—C47—H47	120.6
C1—C2—H2	120.0	C48—C47—H47	120.6
C2—C3—C4	117.9 (5)	C49—C48—C47	118.5 (6)
C2—C3—H3	121.0	C49—C48—H48	120.8
C4—C3—H3	121.0	C47—C48—H48	120.8
C3—C4—C5	119.8 (5)	C48—C49—C50	119.8 (7)
C3—C4—H4	120.1	C48—C49—H49	120.1
C5—C4—H4	120.1	C50—C49—H49	120.1
N1—C5—C4	122.2 (5)	N3—C50—C49	122.2 (6)
N1—C5—H5	118.9	N3—C50—H50	118.9
C4—C5—H5	118.9	C49—C50—H50	118.9
O2—C6—O3	124.3 (4)	O17—C51—O18	124.6 (4)
O2—C6—C7	118.1 (4)	O17—C51—C52	120.2 (4)
O3—C6—C7	117.5 (4)	O18—C51—C52	115.3 (4)
C9C—C7—C10A	69.4 (8)	C53A—C52—C54C	69.1 (7)
C9C—C7—C8A	126.9 (9)	C53A—C52—C55C	129.1 (7)

C10A—C7—C8A	115.1 (8)	C54C—C52—C55C	112.9 (7)
C9C—C7—C6	112.8 (7)	C53A—C52—C55A	114.8 (7)
C10A—C7—C6	114.4 (6)	C54C—C52—C55A	127.9 (7)
C8A—C7—C6	111.7 (6)	C53A—C52—C51	111.0 (6)
C9C—C7—C8C	116.7 (8)	C54C—C52—C51	114.8 (6)
C10A—C7—C8C	126.5 (8)	C55C—C52—C51	112.6 (5)
C6—C7—C8C	110.6 (6)	C55A—C52—C51	111.3 (5)
C9C—C7—C10C	105.0 (8)	C54C—C52—C53C	105.4 (7)
C8A—C7—C10C	90.2 (8)	C55C—C52—C53C	107.4 (6)
C6—C7—C10C	104.6 (6)	C55A—C52—C53C	86.6 (7)
C8C—C7—C10C	105.9 (8)	C51—C52—C53C	102.6 (5)
C10A—C7—C9A	104.8 (7)	C53A—C52—C54A	107.1 (7)
C8A—C7—C9A	107.7 (7)	C55C—C52—C54A	86.1 (6)
C6—C7—C9A	101.9 (5)	C55A—C52—C54A	107.6 (6)
C8C—C7—C9A	92.5 (7)	C51—C52—C54A	104.4 (5)
C10C—C7—C9A	139.5 (7)	C53C—C52—C54A	142.0 (7)
C7—C8A—H8A	109.5	C52—C53A—H53A	109.5
C7—C8A—H8B	109.5	C52—C53A—H53B	109.5
C7—C8A—H8C	109.5	C52—C53A—H53C	109.5
C7—C9A—H9A	109.5	C52—C54A—H54A	109.5
C7—C9A—H9B	109.5	C52—C54A—H54B	109.5
C7—C9A—H9C	109.5	C52—C54A—H54C	109.5
C7—C10A—H10A	109.5	C52—C55A—H55A	109.5
C7—C10A—H10B	109.5	C52—C55A—H55B	109.5
C7—C10A—H10C	109.5	C52—C55A—H55C	109.5
C7—C8C—H8D	109.5	C52—C53C—H53D	109.5
C7—C8C—H8E	109.5	C52—C53C—H53E	109.5
H8D—C8C—H8E	109.5	H53D—C53C—H53E	109.5
C7—C8C—H8F	109.5	C52—C53C—H53F	109.5
H8D—C8C—H8F	109.5	H53D—C53C—H53F	109.5
H8E—C8C—H8F	109.5	H53E—C53C—H53F	109.5
C7—C9C—H9D	109.5	C52—C54C—H54D	109.5
C7—C9C—H9E	109.5	C52—C54C—H54E	109.5
H9D—C9C—H9E	109.5	H54D—C54C—H54E	109.5
C7—C9C—H9F	109.5	C52—C54C—H54F	109.5
H9D—C9C—H9F	109.5	H54D—C54C—H54F	109.5
H9E—C9C—H9F	109.5	H54E—C54C—H54F	109.5
C7—C10C—H10D	109.5	C52—C55C—H55D	109.5
C7—C10C—H10E	109.5	C52—C55C—H55E	109.5
H10D—C10C—H10E	109.5	H55D—C55C—H55E	109.5
C7—C10C—H10F	109.5	C52—C55C—H55F	109.5
H10D—C10C—H10F	109.5	H55D—C55C—H55F	109.5
H10E—C10C—H10F	109.5	H55E—C55C—H55F	109.5
O4—C11—O5	124.7 (4)	O20—C56—O19	124.2 (4)
O4—C11—C12	119.9 (4)	O20—C56—C57	118.4 (4)
O5—C11—C12	115.4 (4)	O19—C56—C57	117.3 (4)
C13—C12—C15	109.4 (5)	C58—C57—C59	110.3 (5)
C13—C12—C11	107.6 (5)	C58—C57—C56	111.4 (4)

C15—C12—C11	110.4 (4)	C59—C57—C56	105.4 (4)
C13—C12—C14	111.3 (5)	C58—C57—C60	110.0 (5)
C15—C12—C14	109.4 (5)	C59—C57—C60	110.0 (4)
C11—C12—C14	108.7 (4)	C56—C57—C60	109.8 (4)
C12—C13—H13A	109.5	C57—C58—H58A	109.5
C12—C13—H13B	109.5	C57—C58—H58B	109.5
H13A—C13—H13B	109.5	H58A—C58—H58B	109.5
C12—C13—H13C	109.5	C57—C58—H58C	109.5
H13A—C13—H13C	109.5	H58A—C58—H58C	109.5
H13B—C13—H13C	109.5	H58B—C58—H58C	109.5
C12—C14—H14A	109.5	C57—C59—H59A	109.5
C12—C14—H14B	109.5	C57—C59—H59B	109.5
H14A—C14—H14B	109.5	H59A—C59—H59B	109.5
C12—C14—H14C	109.5	C57—C59—H59C	109.5
H14A—C14—H14C	109.5	H59A—C59—H59C	109.5
H14B—C14—H14C	109.5	H59B—C59—H59C	109.5
C12—C15—H15A	109.5	C57—C60—H60A	109.5
C12—C15—H15B	109.5	C57—C60—H60B	109.5
H15A—C15—H15B	109.5	H60A—C60—H60B	109.5
C12—C15—H15C	109.5	C57—C60—H60C	109.5
H15A—C15—H15C	109.5	H60A—C60—H60C	109.5
H15B—C15—H15C	109.5	H60B—C60—H60C	109.5
N2—C16—C17	121.7 (5)	N4—C61—C62	122.4 (5)
N2—C16—H16	119.1	N4—C61—H61	118.8
C17—C16—H16	119.1	C62—C61—H61	118.8
C18—C17—C16	119.3 (5)	C63—C62—C61	119.1 (5)
C18—C17—H17	120.4	C63—C62—H62	120.5
C16—C17—H17	120.4	C61—C62—H62	120.5
C17—C18—C19	119.4 (5)	C62—C63—C64	119.2 (5)
C17—C18—H18	120.3	C62—C63—H63	120.4
C19—C18—H18	120.3	C64—C63—H63	120.4
C20—C19—C18	118.6 (5)	C63—C64—C65	119.3 (5)
C20—C19—H19	120.7	C63—C64—H64	120.3
C18—C19—H19	120.7	C65—C64—H64	120.3
N2—C20—C19	122.5 (5)	N4—C65—C64	122.2 (4)
N2—C20—H20	118.7	N4—C65—H65	118.9
C19—C20—H20	118.7	C64—C65—H65	118.9
O6—C21—O7	124.5 (4)	O22—C66—O21	124.7 (4)
O6—C21—C22	116.3 (4)	O22—C66—C67	118.9 (4)
O7—C21—C22	119.2 (4)	O21—C66—C67	116.4 (4)
C24A—C22—C25C	49.7 (8)	C68C—C67—C69A	143.0 (9)
C24A—C22—C23C	126.6 (9)	C68C—C67—C69C	116.1 (9)
C25C—C22—C23C	118.3 (10)	C68C—C67—C66	107.8 (7)
C24A—C22—C21	116.4 (6)	C69A—C67—C66	108.5 (6)
C25C—C22—C21	114.3 (8)	C69C—C67—C66	110.7 (6)
C23C—C22—C21	114.5 (7)	C68C—C67—C70A	58.9 (8)
C24A—C22—C23A	114.2 (7)	C69A—C67—C70A	112.8 (7)
C25C—C22—C23A	132.8 (9)	C69C—C67—C70A	136.4 (7)

C21—C22—C23A	112.0 (5)	C66—C67—C70A	111.6 (5)
C24A—C22—C24C	50.9 (8)	C68C—C67—C70C	111.0 (9)
C25C—C22—C24C	100.5 (9)	C69A—C67—C70C	65.7 (9)
C23C—C22—C24C	103.9 (9)	C69C—C67—C70C	105.3 (9)
C21—C22—C24C	101.9 (8)	C66—C67—C70C	105.4 (8)
C23A—C22—C24C	78.2 (8)	C70A—C67—C70C	53.0 (8)
C24A—C22—C25A	103.6 (6)	C68C—C67—C68A	49.0 (8)
C25C—C22—C25A	55.0 (8)	C69A—C67—C68A	110.6 (7)
C23C—C22—C25A	79.2 (9)	C69C—C67—C68A	70.9 (7)
C21—C22—C25A	103.1 (6)	C66—C67—C68A	109.1 (5)
C23A—C22—C25A	105.9 (6)	C70A—C67—C68A	104.2 (6)
C24C—C22—C25A	150.8 (9)	C70C—C67—C68A	144.3 (9)
C22—C23A—H23A	109.5	C67—C68A—H68A	109.5
C22—C23A—H23B	109.5	C67—C68A—H68B	109.5
C22—C23A—H23C	109.5	C67—C68A—H68C	109.5
C22—C24A—H24A	109.5	C67—C69A—H69A	109.5
C22—C24A—H24B	109.5	C67—C69A—H69B	109.5
C22—C24A—H24C	109.5	C67—C69A—H69C	109.5
C22—C25A—H25A	109.5	C67—C70A—H70A	109.5
C22—C25A—H25B	109.5	C67—C70A—H70B	109.5
C22—C25A—H25C	109.5	C67—C70A—H70C	109.5
C22—C23C—H23D	109.5	C67—C68C—H68D	109.5
C22—C23C—H23E	109.5	C67—C68C—H68E	109.5
H23D—C23C—H23E	109.5	H68D—C68C—H68E	109.5
C22—C23C—H23F	109.5	C67—C68C—H68F	109.5
H23D—C23C—H23F	109.5	H68D—C68C—H68F	109.5
H23E—C23C—H23F	109.5	H68E—C68C—H68F	109.5
C22—C24C—H24D	109.5	C67—C69C—H69D	109.5
C22—C24C—H24E	109.5	C67—C69C—H69E	109.5
H24D—C24C—H24E	109.5	H69D—C69C—H69E	109.5
C22—C24C—H24F	109.5	C67—C69C—H69F	109.5
H24D—C24C—H24F	109.5	H69D—C69C—H69F	109.5
H24E—C24C—H24F	109.5	H69E—C69C—H69F	109.5
C22—C25C—H25D	109.5	C67—C70C—H70D	109.4
C22—C25C—H25E	109.5	C67—C70C—H70E	109.5
H25D—C25C—H25E	109.5	H70D—C70C—H70E	109.5
C22—C25C—H25F	109.5	C67—C70C—H70F	109.5
H25D—C25C—H25F	109.5	H70D—C70C—H70F	109.5
H25E—C25C—H25F	109.5	H70E—C70C—H70F	109.5
O9—C26—O8	124.5 (4)	O23—C71—O24	123.8 (4)
O9—C26—C27	119.7 (4)	O23—C71—C72	118.8 (4)
O8—C26—C27	115.8 (4)	O24—C71—C72	117.4 (4)
C28A—C27—C29C	123.9 (11)	C73—C72—C71	111.0 (4)
C28A—C27—C30C	84.9 (9)	C73—C72—C74	109.4 (4)
C29C—C27—C30C	110.7 (10)	C71—C72—C74	108.8 (4)
C28A—C27—C26	113.0 (7)	C73—C72—C75	109.5 (4)
C29C—C27—C26	112.6 (9)	C71—C72—C75	108.7 (4)
C30C—C27—C26	107.0 (8)	C74—C72—C75	109.3 (4)

C29C—C27—C28C	107.5 (9)	C72—C73—H73A	109.5
C30C—C27—C28C	109.8 (9)	C72—C73—H73B	109.5
C26—C27—C28C	109.3 (7)	H73A—C73—H73B	109.5
C28A—C27—C30A	111.4 (8)	C72—C73—H73C	109.5
C29C—C27—C30A	80.6 (9)	H73A—C73—H73C	109.5
C26—C27—C30A	110.3 (5)	H73B—C73—H73C	109.5
C28C—C27—C30A	132.1 (8)	C72—C74—H74A	109.5
C28A—C27—C29A	113.7 (8)	C72—C74—H74B	109.5
C30C—C27—C29A	132.8 (9)	H74A—C74—H74B	109.5
C26—C27—C29A	104.4 (6)	C72—C74—H74C	109.5
C28C—C27—C29A	91.6 (8)	H74A—C74—H74C	109.5
C30A—C27—C29A	103.4 (7)	H74B—C74—H74C	109.5
C27—C28A—H28A	109.5	C72—C75—H75A	109.5
C27—C28A—H28B	109.5	C72—C75—H75B	109.5
C27—C28A—H28C	109.4	H75A—C75—H75B	109.5
C27—C29A—H29A	109.5	C72—C75—H75C	109.5
C27—C29A—H29B	109.5	H75A—C75—H75C	109.5
C27—C29A—H29C	109.5	H75B—C75—H75C	109.5
C27—C30A—H30A	109.5	O25—C76—O26	121.5 (4)
C27—C30A—H30B	109.5	O25—C76—C77	123.2 (4)
C27—C30A—H30C	109.5	O26—C76—C77	115.2 (4)
C27—C28C—H28D	109.5	C79A—C77—C80A	116.2 (6)
C27—C28C—H28E	109.5	C79A—C77—C78C	67.6 (11)
H28D—C28C—H28E	109.5	C80A—C77—C78C	133.7 (10)
C27—C28C—H28F	109.5	C79A—C77—C80C	130.8 (9)
H28D—C28C—H28F	109.5	C78C—C77—C80C	113.6 (11)
H28E—C28C—H28F	109.5	C79A—C77—C76	113.1 (5)
C27—C29C—H29D	109.5	C80A—C77—C76	108.7 (5)
C27—C29C—H29E	109.5	C78C—C77—C76	111.0 (9)
H29D—C29C—H29E	109.5	C80C—C77—C76	111.5 (8)
C27—C29C—H29F	109.5	C80A—C77—C79C	83.9 (9)
H29D—C29C—H29F	109.5	C78C—C77—C79C	106.3 (10)
H29E—C29C—H29F	109.5	C80C—C77—C79C	107.5 (10)
C27—C30C—H30D	109.5	C76—C77—C79C	106.5 (7)
C27—C30C—H30E	109.5	C79A—C77—C78A	105.7 (5)
H30D—C30C—H30E	109.5	C80A—C77—C78A	109.0 (5)
C27—C30C—H30F	109.5	C80C—C77—C78A	83.1 (10)
H30D—C30C—H30F	109.5	C76—C77—C78A	103.3 (5)
H30E—C30C—H30F	109.5	C79C—C77—C78A	141.5 (9)
O10—C31—O11	123.3 (5)	C77—C78A—H78A	109.5
O10—C31—C32	123.7 (6)	C77—C78A—H78B	109.5
O11—C31—C32	112.9 (6)	C77—C78A—H78C	109.5
C35C—C32—C34A	88.2 (19)	C77—C79A—H79A	109.5
C35C—C32—C31	109.7 (13)	C77—C79A—H79B	109.4
C34A—C32—C31	106.9 (6)	C77—C79A—H79C	109.5
C35C—C32—C33C	112.3 (13)	C77—C80A—H80A	109.5
C34A—C32—C33C	128.3 (11)	C77—C80A—H80B	109.5
C31—C32—C33C	109.2 (7)	C77—C80A—H80C	109.5

C34A—C32—C35A	109.2 (6)	C77—C78C—H78D	110.4
C31—C32—C35A	108.9 (6)	C77—C78C—H78E	110.2
C33C—C32—C35A	92.6 (13)	H78D—C78C—H78E	108.6
C35C—C32—C34C	112.2 (13)	C77—C78C—H78F	110.5
C31—C32—C34C	106.8 (11)	H78D—C78C—H78F	108.5
C33C—C32—C34C	106.6 (11)	H78E—C78C—H78F	108.6
C35A—C32—C34C	130.6 (16)	C77—C79C—H79D	109.5
C35C—C32—C33A	132.6 (15)	C77—C79C—H79E	109.4
C34A—C32—C33A	108.3 (7)	H79D—C79C—H79E	109.5
C31—C32—C33A	107.3 (6)	C77—C79C—H79F	109.5
C35A—C32—C33A	115.9 (7)	H79D—C79C—H79F	109.5
C34C—C32—C33A	83.7 (15)	H79E—C79C—H79F	109.5
C32—C33A—H33A	109.5	C77—C80C—H80D	109.4
C32—C33A—H33B	109.4	C77—C80C—H80E	109.5
C32—C33A—H33C	109.5	H80D—C80C—H80E	109.5
C32—C34A—H34A	109.5	C77—C80C—H80F	109.5
C32—C34A—H34B	109.5	H80D—C80C—H80F	109.5
C32—C34A—H34C	109.4	H80E—C80C—H80F	109.5
C32—C35A—H35A	109.5	O27—C81—O28	124.3 (4)
C32—C35A—H35B	109.5	O27—C81—C82	119.8 (4)
C32—C35A—H35C	109.4	O28—C81—C82	115.8 (4)
C32—C33C—H33D	109.5	C83A—C82—C84C	136.9 (9)
C32—C33C—H33E	109.5	C83A—C82—C85C	67.2 (8)
H33D—C33C—H33E	109.5	C84C—C82—C85C	113.7 (9)
C32—C33C—H33F	109.4	C83A—C82—C81	111.4 (6)
H33D—C33C—H33F	109.5	C84C—C82—C81	108.5 (7)
H33E—C33C—H33F	109.5	C85C—C82—C81	109.2 (6)
C32—C34C—H34D	110.0	C83A—C82—C84A	112.6 (8)
C32—C34C—H34E	109.8	C85C—C82—C84A	140.3 (8)
H34D—C34C—H34E	109.0	C81—C82—C84A	107.3 (6)
C32—C34C—H34F	110.0	C83A—C82—C85A	110.2 (8)
H34D—C34C—H34F	109.0	C84C—C82—C85A	70.4 (8)
H34E—C34C—H34F	109.0	C85C—C82—C85A	46.6 (7)
C32—C35C—H35D	110.0	C81—C82—C85A	108.9 (6)
C32—C35C—H35E	110.0	C84A—C82—C85A	106.3 (7)
H35D—C35C—H35E	109.0	C84C—C82—C83C	109.2 (8)
C32—C35C—H35F	110.0	C85C—C82—C83C	104.8 (8)
H35D—C35C—H35F	109.0	C81—C82—C83C	111.4 (6)
H35E—C35C—H35F	110.0	C84A—C82—C83C	75.3 (7)
O12—C36—O13	123.8 (4)	C85A—C82—C83C	137.0 (8)
O12—C36—C37	119.8 (4)	C82—C83A—H83A	109.5
O13—C36—C37	116.4 (4)	C82—C83A—H83B	109.5
C38—C37—C36	111.4 (5)	C82—C83A—H83C	109.5
C38—C37—C39	110.1 (5)	C82—C84A—H84A	109.5
C36—C37—C39	107.5 (4)	C82—C84A—H84B	109.5
C38—C37—C40	109.7 (4)	C82—C84A—H84C	109.5
C36—C37—C40	108.9 (4)	C82—C85A—H85A	109.5
C39—C37—C40	109.1 (5)	C82—C85A—H85B	109.5

C37—C38—H38A	109.5	C82—C85A—H85C	109.5
C37—C38—H38B	109.5	C82—C83C—H83D	109.5
H38A—C38—H38B	109.5	C82—C83C—H83E	109.5
C37—C38—H38C	109.5	H83D—C83C—H83E	109.5
H38A—C38—H38C	109.5	C82—C83C—H83F	109.5
H38B—C38—H38C	109.5	H83D—C83C—H83F	109.5
C37—C39—H39A	109.5	H83E—C83C—H83F	109.5
C37—C39—H39B	109.5	C82—C84C—H84D	109.5
H39A—C39—H39B	109.5	C82—C84C—H84E	109.5
C37—C39—H39C	109.5	H84D—C84C—H84E	109.5
H39A—C39—H39C	109.5	C82—C84C—H84F	109.5
H39B—C39—H39C	109.5	H84D—C84C—H84F	109.5
C37—C40—H40A	109.5	H84E—C84C—H84F	109.5
C37—C40—H40B	109.5	C82—C85C—H85D	109.5
H40A—C40—H40B	109.5	C82—C85C—H85E	109.5
C37—C40—H40C	109.5	H85D—C85C—H85E	109.5
H40A—C40—H40C	109.5	C82—C85C—H85F	109.5
H40B—C40—H40C	109.5	H85D—C85C—H85F	109.5
O14—C41—O15	124.7 (4)	H85E—C85C—H85F	109.5
O14—C41—C42	119.6 (4)	O29—C86—O30	124.1 (4)
O15—C41—C42	115.7 (4)	O29—C86—C87	119.4 (4)
C44C—C42—C43A	128.6 (9)	O30—C86—C87	116.5 (4)
C44C—C42—C41	115.0 (8)	C89A—C87—C88C	72.6 (8)
C43A—C42—C41	115.7 (6)	C89A—C87—C90C	127.7 (9)
C44C—C42—C45A	53.7 (8)	C88C—C87—C90C	110.7 (8)
C43A—C42—C45A	115.7 (8)	C89A—C87—C86	111.7 (6)
C41—C42—C45A	108.0 (6)	C88C—C87—C86	111.3 (6)
C44C—C42—C43C	113.5 (10)	C90C—C87—C86	114.4 (7)
C41—C42—C43C	109.4 (8)	C89A—C87—C90A	114.0 (7)
C45A—C42—C43C	142.0 (10)	C88C—C87—C90A	131.5 (6)
C44C—C42—C45C	109.3 (10)	C86—C87—C90A	109.8 (5)
C43A—C42—C45C	67.4 (9)	C89A—C87—C88A	108.4 (7)
C41—C42—C45C	102.4 (8)	C90C—C87—C88A	82.8 (8)
C45A—C42—C45C	58.6 (9)	C86—C87—C88A	104.4 (5)
C43C—C42—C45C	106.3 (10)	C90A—C87—C88A	108.1 (6)
C44C—C42—C44A	46.4 (8)	C88C—C87—C89C	104.9 (8)
C43A—C42—C44A	110.2 (7)	C90C—C87—C89C	109.4 (8)
C41—C42—C44A	105.6 (6)	C86—C87—C89C	105.5 (6)
C45A—C42—C44A	100.1 (7)	C90A—C87—C89C	87.7 (7)
C43C—C42—C44A	76.0 (9)	C88A—C87—C89C	138.7 (8)
C45C—C42—C44A	149.2 (9)	C87—C88A—H88A	109.5
C42—C43A—H43A	109.5	C87—C88A—H88B	109.5
C42—C43A—H43B	109.5	C87—C88A—H88C	109.5
C42—C43A—H43C	109.5	C87—C89A—H89A	109.5
C42—C44A—H44A	109.5	C87—C89A—H89B	109.5
C42—C44A—H44B	109.5	C87—C89A—H89C	109.5
C42—C44A—H44C	109.5	C87—C90A—H90A	109.5
C42—C45A—H45A	109.5	C87—C90A—H90B	109.5

C42—C45A—H45B	109.5	C87—C90A—H90C	109.5
C42—C45A—H45C	109.5	C87—C88C—H88D	109.5
C42—C43C—H43D	109.5	C87—C88C—H88E	109.5
C42—C43C—H43E	109.5	H88D—C88C—H88E	109.5
H43D—C43C—H43E	109.5	C87—C88C—H88F	109.5
C42—C43C—H43F	109.5	H88D—C88C—H88F	109.5
H43D—C43C—H43F	109.5	H88E—C88C—H88F	109.5
H43E—C43C—H43F	109.5	C87—C89C—H89D	109.5
C42—C44C—H44D	109.5	C87—C89C—H89E	109.5
C42—C44C—H44E	109.5	H89D—C89C—H89E	109.5
H44D—C44C—H44E	109.5	C87—C89C—H89F	109.5
C42—C44C—H44F	109.5	H89D—C89C—H89F	109.5
H44D—C44C—H44F	109.5	H89E—C89C—H89F	109.5
H44E—C44C—H44F	109.5	C87—C90C—H90D	109.5
C42—C45C—H45D	109.5	C87—C90C—H90E	109.5
C42—C45C—H45E	109.5	H90D—C90C—H90E	109.5
H45D—C45C—H45E	109.5	C87—C90C—H90F	109.5
C42—C45C—H45F	109.5	H90D—C90C—H90F	109.5
H45D—C45C—H45F	109.5	H90E—C90C—H90F	109.5
H45E—C45C—H45F	109.5		

O5—Mn1A—Mn2A—O1	−127.6 (2)	O28—Mn1B—Mn2B—O16	62.9 (2)
O15—Mn1A—Mn2A—O1	64.1 (2)	O19—Mn1B—Mn2B—O16	−123.2 (2)
O13—Mn1A—Mn2A—O1	−46.1 (2)	N3—Mn1B—Mn2B—O16	−179.9 (3)
N1—Mn1A—Mn2A—O1	177.6 (3)	O30—Mn1B—Mn2B—O16	−41.2 (2)
O2—Mn1A—Mn2A—O1	142.3 (2)	O17—Mn1B—Mn2B—O16	140.3 (2)
O1—Mn1A—Mn2A—O8	60.6 (2)	O16—Mn1B—Mn2B—O21	56.3 (2)
O5—Mn1A—Mn2A—O8	−67.00 (14)	O28—Mn1B—Mn2B—O21	119.19 (13)
O15—Mn1A—Mn2A—O8	124.70 (13)	O19—Mn1B—Mn2B—O21	−66.97 (13)
O13—Mn1A—Mn2A—O8	14.47 (14)	N3—Mn1B—Mn2B—O21	−123.6 (3)
N1—Mn1A—Mn2A—O8	−121.9 (3)	O30—Mn1B—Mn2B—O21	15.03 (14)
O2—Mn1A—Mn2A—O8	−157.16 (14)	O17—Mn1B—Mn2B—O21	−163.41 (12)
O1—Mn1A—Mn2A—O3	−124.7 (2)	O16—Mn1B—Mn2B—O18	−124.9 (2)
O5—Mn1A—Mn2A—O3	107.75 (13)	O28—Mn1B—Mn2B—O18	−61.95 (13)
O15—Mn1A—Mn2A—O3	−60.55 (13)	O19—Mn1B—Mn2B—O18	111.90 (12)
O13—Mn1A—Mn2A—O3	−170.79 (14)	N3—Mn1B—Mn2B—O18	55.2 (3)
N1—Mn1A—Mn2A—O3	52.9 (3)	O30—Mn1B—Mn2B—O18	−166.11 (13)
O2—Mn1A—Mn2A—O3	17.59 (13)	O17—Mn1B—Mn2B—O18	15.45 (12)
O1—Mn1A—Mn2A—N2	177.1 (3)	O16—Mn1B—Mn2B—N4	176.6 (3)
O5—Mn1A—Mn2A—N2	49.5 (2)	O28—Mn1B—Mn2B—N4	−120.5 (2)
O15—Mn1A—Mn2A—N2	−118.8 (2)	O19—Mn1B—Mn2B—N4	53.4 (2)
O13—Mn1A—Mn2A—N2	131.0 (2)	N3—Mn1B—Mn2B—N4	−3.3 (3)
N1—Mn1A—Mn2A—N2	−5.4 (3)	O30—Mn1B—Mn2B—N4	135.3 (2)
O2—Mn1A—Mn2A—N2	−40.6 (2)	O17—Mn1B—Mn2B—N4	−43.1 (2)
O1—Mn1A—Mn2A—O6	−43.8 (2)	O16—Mn1B—Mn2B—O20	137.8 (2)
O5—Mn1A—Mn2A—O6	−171.38 (14)	O28—Mn1B—Mn2B—O20	−159.25 (12)
O15—Mn1A—Mn2A—O6	20.31 (14)	O19—Mn1B—Mn2B—O20	14.60 (12)
O13—Mn1A—Mn2A—O6	−89.92 (14)	N3—Mn1B—Mn2B—O20	−42.1 (3)

N1—Mn1A—Mn2A—O6	133.7 (3)
O2—Mn1A—Mn2A—O6	98.46 (14)
O1—Mn1A—Mn2A—O4	143.6 (2)
O5—Mn1A—Mn2A—O4	15.99 (13)
O15—Mn1A—Mn2A—O4	−152.32 (13)
O13—Mn1A—Mn2A—O4	97.45 (13)
N1—Mn1A—Mn2A—O4	−38.9 (3)
O2—Mn1A—Mn2A—O4	−74.17 (13)
O5—Mn1A—O1—Mn2A	51.7 (2)
O15—Mn1A—O1—Mn2A	−120.47 (18)
O13—Mn1A—O1—Mn2A	139.99 (18)
O2—Mn1A—O1—Mn2A	−36.05 (19)
O5—Mn1A—O1—Mn3A	−127.73 (16)
O15—Mn1A—O1—Mn3A	60.09 (16)
O13—Mn1A—O1—Mn3A	−39.46 (17)
O2—Mn1A—O1—Mn3A	144.50 (15)
Mn2A—Mn1A—O1—Mn3A	−179.4 (3)
O8—Mn2A—O1—Mn1A	−124.74 (19)
O3—Mn2A—O1—Mn1A	54.05 (19)
O6—Mn2A—O1—Mn1A	142.33 (18)
O4—Mn2A—O1—Mn1A	−34.86 (19)
O8—Mn2A—O1—Mn3A	54.70 (17)
O3—Mn2A—O1—Mn3A	−126.52 (17)
O6—Mn2A—O1—Mn3A	−38.23 (18)
O4—Mn2A—O1—Mn3A	144.58 (16)
Mn1A—Mn2A—O1—Mn3A	179.4 (3)
O12—Mn3A—O1—Mn1A	51.80 (17)
O9—Mn3A—O1—Mn1A	141.47 (17)
O14—Mn3A—O1—Mn1A	−47.39 (17)
O7—Mn3A—O1—Mn1A	−132.66 (17)
O12—Mn3A—O1—Mn2A	−127.66 (17)
O9—Mn3A—O1—Mn2A	−37.99 (18)
O14—Mn3A—O1—Mn2A	133.14 (17)
O7—Mn3A—O1—Mn2A	47.88 (18)
O1—Mn1A—O2—C6	−7.1 (4)
O5—Mn1A—O2—C6	−104.1 (4)
O15—Mn1A—O2—C6	85.4 (4)
O13—Mn1A—O2—C6	−169.3 (5)
N1—Mn1A—O2—C6	170.8 (4)
Mn2A—Mn1A—O2—C6	−24.4 (3)
O1—Mn2A—O3—C6	−45.5 (4)
N2—Mn2A—O3—C6	133.2 (4)
O6—Mn2A—O3—C6	−142.1 (4)
O4—Mn2A—O3—C6	50.8 (4)
Mn1A—Mn2A—O3—C6	−22.1 (3)
O1—Mn2A—O4—C11	1.2 (4)
O8—Mn2A—O4—C11	95.4 (4)
O3—Mn2A—O4—C11	−94.0 (4)
O30—Mn1B—Mn2B—O20	96.59 (13)
O17—Mn1B—Mn2B—O20	−81.85 (12)
O16—Mn1B—Mn2B—O23	−46.7 (2)
O28—Mn1B—Mn2B—O23	16.18 (13)
O19—Mn1B—Mn2B—O23	−169.98 (12)
N3—Mn1B—Mn2B—O23	133.4 (3)
O30—Mn1B—Mn2B—O23	−87.99 (13)
O17—Mn1B—Mn2B—O23	93.57 (12)
O21—Mn2B—O16—Mn1B	−129.50 (18)
O18—Mn2B—O16—Mn1B	53.86 (19)
O20—Mn2B—O16—Mn1B	−39.53 (18)
O23—Mn2B—O16—Mn1B	139.14 (17)
O21—Mn2B—O16—Mn3B	49.12 (16)
O18—Mn2B—O16—Mn3B	−127.52 (15)
O20—Mn2B—O16—Mn3B	139.09 (15)
O23—Mn2B—O16—Mn3B	−42.24 (16)
Mn1B—Mn2B—O16—Mn3B	178.6 (3)
O28—Mn1B—O16—Mn2B	−122.75 (18)
O19—Mn1B—O16—Mn2B	55.68 (19)
O30—Mn1B—O16—Mn2B	144.69 (17)
O17—Mn1B—O16—Mn2B	−37.58 (18)
O28—Mn1B—O16—Mn3B	58.58 (16)
O19—Mn1B—O16—Mn3B	−123.00 (14)
O30—Mn1B—O16—Mn3B	−33.98 (16)
O17—Mn1B—O16—Mn3B	143.75 (14)
Mn2B—Mn1B—O16—Mn3B	−178.7 (3)
O29—Mn3B—O16—Mn2B	−128.48 (16)
O22—Mn3B—O16—Mn2B	−35.42 (17)
O27—Mn3B—O16—Mn2B	139.70 (16)
O24—Mn3B—O16—Mn2B	54.88 (16)
O29—Mn3B—O16—Mn1B	50.25 (16)
O22—Mn3B—O16—Mn1B	143.32 (15)
O27—Mn3B—O16—Mn1B	−41.56 (16)
O24—Mn3B—O16—Mn1B	−126.38 (15)
O16—Mn1B—O17—C51	−8.7 (3)
O28—Mn1B—O17—C51	87.0 (3)
O19—Mn1B—O17—C51	−104.1 (3)
N3—Mn1B—O17—C51	172.0 (4)
O30—Mn1B—O17—C51	160.5 (5)
Mn2B—Mn1B—O17—C51	−26.0 (3)
O16—Mn2B—O18—C51	−37.8 (4)
O21—Mn2B—O18—C51	159.4 (6)
N4—Mn2B—O18—C51	138.5 (4)
O20—Mn2B—O18—C51	55.0 (3)
O23—Mn2B—O18—C51	−134.0 (3)
Mn1B—Mn2B—O18—C51	−15.2 (3)
O16—Mn1B—O19—C56	−33.2 (3)
O28—Mn1B—O19—C56	138.8 (6)

N2—Mn2A—O4—C11	−179.7 (4)	N3—Mn1B—O19—C56	145.9 (4)
O6—Mn2A—O4—C11	−166.8 (5)	O30—Mn1B—O19—C56	−130.8 (3)
Mn1A—Mn2A—O4—C11	−15.5 (4)	O17—Mn1B—O19—C56	61.2 (3)
O1—Mn1A—O5—C11	−49.2 (4)	Mn2B—Mn1B—O19—C56	−10.2 (3)
O15—Mn1A—O5—C11	93.4 (6)	O16—Mn2B—O20—C56	−10.5 (3)
O13—Mn1A—O5—C11	−145.1 (4)	O21—Mn2B—O20—C56	85.4 (3)
N1—Mn1A—O5—C11	131.7 (4)	O18—Mn2B—O20—C56	−105.6 (3)
O2—Mn1A—O5—C11	46.7 (3)	N4—Mn2B—O20—C56	170.3 (4)
Mn2A—Mn1A—O5—C11	−26.5 (3)	Mn1B—Mn2B—O20—C56	−28.7 (3)
O1—Mn2A—O6—C21	11.1 (5)	O16—Mn2B—O21—C66	−49.1 (4)
O8—Mn2A—O6—C21	−83.5 (5)	O18—Mn2B—O21—C66	113.7 (7)
O3—Mn2A—O6—C21	106.2 (5)	N4—Mn2B—O21—C66	134.6 (4)
N2—Mn2A—O6—C21	−168.1 (5)	O20—Mn2B—O21—C66	−141.6 (4)
O4—Mn2A—O6—C21	179.1 (5)	O23—Mn2B—O21—C66	47.6 (4)
Mn1A—Mn2A—O6—C21	30.7 (5)	Mn1B—Mn2B—O21—C66	−72.0 (4)
O1—Mn3A—O7—C21	−36.2 (4)	O16—Mn3B—O22—C66	3.9 (4)
O9—Mn3A—O7—C21	54.4 (4)	O29—Mn3B—O22—C66	102.5 (4)
O14—Mn3A—O7—C21	−125.3 (4)	O24—Mn3B—O22—C66	−86.2 (4)
O10—Mn3A—O7—C21	151.3 (4)	O25—Mn3B—O22—C66	−168.1 (4)
O1—Mn2A—O8—C26	−45.0 (4)	O16—Mn2B—O23—C71	−5.0 (4)
N2—Mn2A—O8—C26	136.3 (4)	O21—Mn2B—O23—C71	−101.0 (4)
O6—Mn2A—O8—C26	52.0 (4)	O18—Mn2B—O23—C71	89.4 (4)
O4—Mn2A—O8—C26	−141.5 (4)	N4—Mn2B—O23—C71	174.2 (4)
Mn1A—Mn2A—O8—C26	−69.8 (4)	Mn1B—Mn2B—O23—C71	14.9 (4)
O1—Mn3A—O9—C26	−8.6 (4)	O16—Mn3B—O24—C71	−35.9 (4)
O12—Mn3A—O9—C26	85.1 (4)	O22—Mn3B—O24—C71	57.1 (4)
O7—Mn3A—O9—C26	−103.7 (4)	O27—Mn3B—O24—C71	−127.6 (4)
O10—Mn3A—O9—C26	170.9 (4)	O25—Mn3B—O24—C71	149.9 (4)
O12—Mn3A—O10—C31	−154.7 (5)	O29—Mn3B—O25—C76	−139.2 (4)
O9—Mn3A—O10—C31	116.2 (5)	O22—Mn3B—O25—C76	128.3 (4)
O14—Mn3A—O10—C31	−54.9 (5)	O27—Mn3B—O25—C76	−47.5 (4)
O7—Mn3A—O10—C31	30.9 (5)	O24—Mn3B—O25—C76	38.4 (4)
O1—Mn3A—O12—C36	−28.2 (4)	O16—Mn3B—O27—C81	0.0 (4)
O9—Mn3A—O12—C36	−119.1 (4)	O29—Mn3B—O27—C81	−98.5 (4)
O14—Mn3A—O12—C36	62.0 (4)	O24—Mn3B—O27—C81	89.9 (4)
O10—Mn3A—O12—C36	144.3 (4)	O25—Mn3B—O27—C81	172.5 (4)
O1—Mn1A—O13—C36	−6.3 (4)	O16—Mn1B—O28—C81	−51.5 (4)
O5—Mn1A—O13—C36	90.7 (4)	O19—Mn1B—O28—C81	136.5 (6)
O15—Mn1A—O13—C36	−100.4 (4)	N3—Mn1B—O28—C81	129.4 (4)
N1—Mn1A—O13—C36	175.9 (4)	O30—Mn1B—O28—C81	46.5 (4)
O2—Mn1A—O13—C36	156.0 (5)	O17—Mn1B—O28—C81	−145.0 (4)
Mn2A—Mn1A—O13—C36	14.2 (4)	Mn2B—Mn1B—O28—C81	−76.1 (4)
O1—Mn3A—O14—C41	−7.3 (4)	O16—Mn3B—O29—C86	−44.2 (3)
O12—Mn3A—O14—C41	−101.0 (4)	O22—Mn3B—O29—C86	−137.7 (3)
O7—Mn3A—O14—C41	87.9 (4)	O27—Mn3B—O29—C86	47.7 (3)
O10—Mn3A—O14—C41	174.4 (4)	O25—Mn3B—O29—C86	129.5 (3)
O1—Mn1A—O15—C41	−32.1 (4)	O16—Mn1B—O30—C86	1.5 (5)
O5—Mn1A—O15—C41	−175.0 (5)	O28—Mn1B—O30—C86	−94.8 (4)

O13—Mn1A—O15—C41	64.7 (4)	O19—Mn1B—O30—C86	96.5 (4)
N1—Mn1A—O15—C41	146.7 (4)	N3—Mn1B—O30—C86	−179.2 (5)
O2—Mn1A—O15—C41	−128.0 (4)	O17—Mn1B—O30—C86	−167.6 (5)
Mn2A—Mn1A—O15—C41	−57.9 (4)	Mn2B—Mn1B—O30—C86	19.5 (5)
O5—Mn1A—N1—C5	−136.2 (3)	O28—Mn1B—N3—C50	−136.2 (4)
O15—Mn1A—N1—C5	35.8 (3)	O19—Mn1B—N3—C50	45.2 (4)
O13—Mn1A—N1—C5	135.7 (3)	O30—Mn1B—N3—C50	−43.9 (4)
O2—Mn1A—N1—C5	−48.7 (3)	O17—Mn1B—N3—C50	138.6 (4)
Mn2A—Mn1A—N1—C5	−82.4 (4)	Mn2B—Mn1B—N3—C50	100.8 (4)
O5—Mn1A—N1—C1	45.1 (3)	O28—Mn1B—N3—C46	42.8 (4)
O15—Mn1A—N1—C1	−142.9 (4)	O19—Mn1B—N3—C46	−135.8 (4)
O13—Mn1A—N1—C1	−43.1 (3)	O30—Mn1B—N3—C46	135.2 (4)
O2—Mn1A—N1—C1	132.5 (4)	O17—Mn1B—N3—C46	−42.4 (4)
Mn2A—Mn1A—N1—C1	98.8 (4)	Mn2B—Mn1B—N3—C46	−80.1 (4)
O8—Mn2A—N2—C16	−139.0 (4)	O21—Mn2B—N4—C65	−133.8 (4)
O3—Mn2A—N2—C16	42.0 (4)	O18—Mn2B—N4—C65	42.2 (4)
O6—Mn2A—N2—C16	−46.1 (4)	O20—Mn2B—N4—C65	136.0 (4)
O4—Mn2A—N2—C16	130.9 (4)	O23—Mn2B—N4—C65	−42.8 (4)
Mn1A—Mn2A—N2—C16	98.7 (4)	Mn1B—Mn2B—N4—C65	99.3 (4)
O8—Mn2A—N2—C20	40.9 (3)	O21—Mn2B—N4—C61	51.3 (3)
O3—Mn2A—N2—C20	−138.1 (4)	O18—Mn2B—N4—C61	−132.7 (3)
O6—Mn2A—N2—C20	133.8 (4)	O20—Mn2B—N4—C61	−39.0 (3)
O4—Mn2A—N2—C20	−49.2 (3)	O23—Mn2B—N4—C61	142.3 (3)
Mn1A—Mn2A—N2—C20	−81.4 (4)	Mn1B—Mn2B—N4—C61	−75.6 (4)
C5—N1—C1—C2	−0.4 (7)	C50—N3—C46—C47	0.1 (8)
Mn1A—N1—C1—C2	178.4 (4)	Mn1B—N3—C46—C47	−179.0 (4)
N1—C1—C2—C3	0.2 (8)	N3—C46—C47—C48	−0.6 (9)
C1—C2—C3—C4	−0.6 (9)	C46—C47—C48—C49	0.4 (10)
C2—C3—C4—C5	1.2 (8)	C47—C48—C49—C50	0.1 (10)
C1—N1—C5—C4	1.0 (7)	C46—N3—C50—C49	0.5 (8)
Mn1A—N1—C5—C4	−177.7 (4)	Mn1B—N3—C50—C49	179.6 (4)
C3—C4—C5—N1	−1.5 (8)	C48—C49—C50—N3	−0.6 (9)
Mn1A—O2—C6—O3	18.7 (7)	Mn1B—O17—C51—O18	26.7 (6)
Mn1A—O2—C6—C7	−165.5 (3)	Mn1B—O17—C51—C52	−154.4 (3)
Mn2A—O3—C6—O2	12.3 (7)	Mn2B—O18—C51—O17	0.8 (6)
Mn2A—O3—C6—C7	−163.5 (3)	Mn2B—O18—C51—C52	−178.3 (3)
O2—C6—C7—C9C	−114.0 (10)	O17—C51—C52—C53A	128.3 (7)
O3—C6—C7—C9C	62.0 (10)	O18—C51—C52—C53A	−52.6 (8)
O2—C6—C7—C10A	169.1 (7)	O17—C51—C52—C54C	−155.8 (8)
O3—C6—C7—C10A	−14.9 (9)	O18—C51—C52—C54C	23.3 (8)
O2—C6—C7—C8A	36.2 (9)	O17—C51—C52—C55C	−24.8 (8)
O3—C6—C7—C8A	−147.8 (7)	O18—C51—C52—C55C	154.3 (6)
O2—C6—C7—C8C	18.8 (9)	O17—C51—C52—C55A	−0.8 (8)
O3—C6—C7—C8C	−165.2 (7)	O18—C51—C52—C55A	178.3 (6)
O2—C6—C7—C10C	132.4 (8)	O17—C51—C52—C53C	90.4 (7)
O3—C6—C7—C10C	−51.6 (8)	O18—C51—C52—C53C	−90.5 (6)
O2—C6—C7—C9A	−78.4 (7)	O17—C51—C52—C54A	−116.6 (6)
O3—C6—C7—C9A	97.6 (6)	O18—C51—C52—C54A	62.5 (6)

Mn2A—O4—C11—O5	2.5 (7)	Mn2B—O20—C56—O19	33.7 (6)
Mn2A—O4—C11—C12	−177.5 (3)	Mn2B—O20—C56—C57	−144.1 (3)
Mn1A—O5—C11—O4	25.2 (6)	Mn1B—O19—C56—O20	−7.3 (6)
Mn1A—O5—C11—C12	−154.8 (3)	Mn1B—O19—C56—C57	170.5 (3)
O4—C11—C12—C13	110.8 (5)	O20—C56—C57—C58	−160.7 (4)
O5—C11—C12—C13	−69.1 (5)	O19—C56—C57—C58	21.4 (6)
O4—C11—C12—C15	−8.5 (7)	O20—C56—C57—C59	79.8 (5)
O5—C11—C12—C15	171.5 (4)	O19—C56—C57—C59	−98.2 (5)
O4—C11—C12—C14	−128.5 (5)	O20—C56—C57—C60	−38.6 (6)
O5—C11—C12—C14	51.5 (6)	O19—C56—C57—C60	143.4 (4)
C20—N2—C16—C17	−0.3 (7)	C65—N4—C61—C62	−1.5 (7)
Mn2A—N2—C16—C17	179.7 (4)	Mn2B—N4—C61—C62	173.6 (4)
N2—C16—C17—C18	−0.7 (8)	N4—C61—C62—C63	1.0 (8)
C16—C17—C18—C19	1.6 (8)	C61—C62—C63—C64	0.3 (8)
C17—C18—C19—C20	−1.5 (8)	C62—C63—C64—C65	−1.0 (8)
C16—N2—C20—C19	0.3 (7)	C61—N4—C65—C64	0.8 (7)
Mn2A—N2—C20—C19	−179.6 (4)	Mn2B—N4—C65—C64	−174.2 (4)
C18—C19—C20—N2	0.6 (8)	C63—C64—C65—N4	0.4 (8)
Mn2A—O6—C21—O7	1.1 (8)	Mn3B—O22—C66—O21	1.8 (7)
Mn2A—O6—C21—C22	177.6 (4)	Mn3B—O22—C66—C67	−179.6 (3)
Mn3A—O7—C21—O6	15.8 (7)	Mn2B—O21—C66—O22	24.8 (7)
Mn3A—O7—C21—C22	−160.6 (4)	Mn2B—O21—C66—C67	−153.8 (3)
O6—C21—C22—C24A	−178.6 (6)	O22—C66—C67—C68C	95.4 (9)
O7—C21—C22—C24A	−2.0 (8)	O21—C66—C67—C68C	−85.9 (9)
O6—C21—C22—C25C	−123.2 (10)	O22—C66—C67—C69A	−92.2 (7)
O7—C21—C22—C25C	53.4 (10)	O21—C66—C67—C69A	86.5 (7)
O6—C21—C22—C23C	17.9 (11)	O22—C66—C67—C69C	−136.6 (8)
O7—C21—C22—C23C	−165.5 (9)	O21—C66—C67—C69C	42.1 (8)
O6—C21—C22—C23A	47.4 (8)	O22—C66—C67—C70A	32.6 (7)
O7—C21—C22—C23A	−135.9 (6)	O21—C66—C67—C70A	−148.7 (5)
O6—C21—C22—C24C	129.4 (9)	O22—C66—C67—C70C	−23.2 (10)
O7—C21—C22—C24C	−54.0 (9)	O21—C66—C67—C70C	155.4 (9)
O6—C21—C22—C25A	−66.0 (6)	O22—C66—C67—C68A	147.2 (6)
O7—C21—C22—C25A	110.6 (6)	O21—C66—C67—C68A	−34.1 (7)
Mn3A—O9—C26—O8	25.4 (7)	Mn2B—O23—C71—O24	28.0 (6)
Mn3A—O9—C26—C27	−154.1 (4)	Mn2B—O23—C71—C72	−150.9 (3)
Mn2A—O8—C26—O9	6.3 (7)	Mn3B—O24—C71—O23	−0.4 (6)
Mn2A—O8—C26—C27	−174.2 (3)	Mn3B—O24—C71—C72	178.6 (3)
O9—C26—C27—C28A	−8.8 (10)	O23—C71—C72—C73	−0.9 (6)
O8—C26—C27—C28A	171.6 (8)	O24—C71—C72—C73	−179.9 (4)
O9—C26—C27—C29C	137.7 (11)	O23—C71—C72—C74	−121.4 (4)
O8—C26—C27—C29C	−41.9 (11)	O24—C71—C72—C74	59.6 (5)
O9—C26—C27—C30C	−100.4 (10)	O23—C71—C72—C75	119.6 (4)
O8—C26—C27—C30C	79.9 (10)	O24—C71—C72—C75	−59.4 (5)
O9—C26—C27—C28C	18.3 (10)	Mn3B—O25—C76—O26	−26.9 (7)
O8—C26—C27—C28C	−161.3 (8)	Mn3B—O25—C76—C77	155.2 (3)
O9—C26—C27—C30A	−134.2 (6)	O25—C76—C77—C79A	−166.1 (6)
O8—C26—C27—C30A	46.2 (7)	O26—C76—C77—C79A	15.9 (7)

O9—C26—C27—C29A	115.2 (7)	O25—C76—C77—C80A	−35.5 (7)
O8—C26—C27—C29A	−64.4 (7)	O26—C76—C77—C80A	146.5 (6)
Mn3A—O10—C31—O11	−26.3 (10)	O25—C76—C77—C78C	120.2 (14)
Mn3A—O10—C31—C32	156.9 (4)	O26—C76—C77—C78C	−57.8 (14)
O10—C31—C32—C35C	−156 (2)	O25—C76—C77—C80C	−7.6 (12)
O11—C31—C32—C35C	26 (2)	O26—C76—C77—C80C	174.5 (11)
O10—C31—C32—C34A	109.3 (8)	O25—C76—C77—C79C	−124.6 (11)
O11—C31—C32—C34A	−67.8 (9)	O26—C76—C77—C79C	57.5 (11)
O10—C31—C32—C33C	−33.0 (16)	O25—C76—C77—C78A	80.2 (6)
O11—C31—C32—C33C	149.8 (15)	O26—C76—C77—C78A	−97.8 (5)
O10—C31—C32—C35A	−132.8 (7)	Mn3B—O27—C81—O28	14.1 (7)
O11—C31—C32—C35A	50.0 (8)	Mn3B—O27—C81—C82	−166.7 (3)
O10—C31—C32—C34C	82 (2)	Mn1B—O28—C81—O27	15.1 (7)
O11—C31—C32—C34C	−95.3 (19)	Mn1B—O28—C81—C82	−164.1 (3)
O10—C31—C32—C33A	−6.6 (10)	O27—C81—C82—C83A	127.5 (8)
O11—C31—C32—C33A	176.3 (8)	O28—C81—C82—C83A	−53.2 (9)
Mn3A—O12—C36—O13	−9.7 (7)	O27—C81—C82—C84C	−69.2 (9)
Mn3A—O12—C36—C37	167.9 (3)	O28—C81—C82—C84C	110.1 (9)
Mn1A—O13—C36—O12	35.0 (7)	O27—C81—C82—C85C	55.2 (9)
Mn1A—O13—C36—C37	−142.7 (4)	O28—C81—C82—C85C	−125.5 (8)
O12—C36—C37—C38	8.5 (6)	O27—C81—C82—C84A	−108.8 (7)
O13—C36—C37—C38	−173.6 (4)	O28—C81—C82—C84A	70.4 (7)
O12—C36—C37—C39	−112.2 (5)	O27—C81—C82—C85A	5.8 (8)
O13—C36—C37—C39	65.6 (5)	O28—C81—C82—C85A	−174.9 (7)
O12—C36—C37—C40	129.7 (5)	O27—C81—C82—C83C	170.5 (8)
O13—C36—C37—C40	−52.5 (6)	O28—C81—C82—C83C	−10.2 (9)
Mn3A—O14—C41—O15	40.2 (7)	Mn3B—O29—C86—O30	18.7 (6)
Mn3A—O14—C41—C42	−141.2 (4)	Mn3B—O29—C86—C87	−161.7 (3)
Mn1A—O15—C41—O14	−18.3 (7)	Mn1B—O30—C86—O29	8.2 (7)
Mn1A—O15—C41—C42	163.0 (4)	Mn1B—O30—C86—C87	−171.4 (3)
O14—C41—C42—C44C	−7.4 (11)	O29—C86—C87—C89A	159.5 (8)
O15—C41—C42—C44C	171.3 (10)	O30—C86—C87—C89A	−20.9 (8)
O14—C41—C42—C43A	−178.4 (7)	O29—C86—C87—C88C	−121.4 (8)
O15—C41—C42—C43A	0.4 (9)	O30—C86—C87—C88C	58.2 (8)
O14—C41—C42—C45A	50.2 (8)	O29—C86—C87—C90C	5.0 (9)
O15—C41—C42—C45A	−131.0 (7)	O30—C86—C87—C90C	−175.4 (8)
O14—C41—C42—C43C	−136.6 (10)	O29—C86—C87—C90A	32.1 (7)
O15—C41—C42—C43C	42.2 (10)	O30—C86—C87—C90A	−148.2 (6)
O14—C41—C42—C45C	111.0 (10)	O29—C86—C87—C88A	−83.6 (7)
O15—C41—C42—C45C	−70.3 (10)	O30—C86—C87—C88A	96.1 (6)
O14—C41—C42—C44A	−56.2 (8)	O29—C86—C87—C89C	125.3 (8)
O15—C41—C42—C44A	122.5 (7)	O30—C86—C87—C89C	−55.1 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H11···O7	0.84	1.77	2.605 (5)	172
O26—H26···O24	0.84	1.73	2.560 (4)	170