metal-organic compounds

 $\nu = 115.826 \ (1)^{\circ}$

Z = 2

V = 2324.7 (2) Å³

Mo $K\alpha$ radiation

 $0.15 \times 0.12 \times 0.10 \text{ mm}$

11959 measured reflections

8138 independent reflections

6183 reflections with $I > 2\sigma(I)$

H-atom parameters constrained

 $\mu = 0.68 \text{ mm}^{-1}$

T = 173 K

 $R_{\rm int} = 0.021$

627 parameters

 $\Delta \rho_{\text{max}} = 0.49 \text{ e } \text{\AA}^{-3}$ $\Delta \rho_{\text{min}} = -0.68 \text{ e } \text{\AA}^{-3}$

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Bis[µ-2-(2-benzoylhydrazinylidenemethyl)-6-methoxyphenolato][2-(2benzoylhydrazinylidenemethyl)-6methoxyphenolato]dimanganese(II) perchlorate methanol solvate

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Key indicators: single-crystal X-ray study; T = 173 K; mean σ (C–C) = 0.006 Å; R factor = 0.045; wR factor = 0.123; data-to-parameter ratio = 13.0.

In the title complex, $[Mn_2(C_{15}H_{13}N_2O_3)_3]ClO_4 \cdot CH_3OH$, the two Mn^{II} ions are bridged by two phenolate O atoms from two ligands, forming an Mn_2O_2 quadrangle. Each Mn^{II} ion has a distorted octahedral coordination geometry. One Mn^{II} ion is coordinated by two N atoms and four O atoms from two ligands, and the other is coordinated by one N atom and five O atoms from three ligands. A dimer is formed by intermolecular $N-H\cdots O$ hydrogen bonds. The dimers, perchlorate anions and methanol solvent molecules are further connected into a chain along [101] through $N-H\cdots O$ and $O-H\cdots O$ hydrogen bonds.

Related literature

For general background to the study of Schiff base compounds, see: Ando *et al.* (2004); Costes *et al.* (1995); Duda *et al.* (2003); Siddall *et al.* (1983). For related structures, see: Li *et al.* (2010); Huang & Li (2007); Mikuriya *et al.* (1992); Yin (2008); Yu *et al.* (2006). For the ligand synthesis, see: Pouralimardan *et al.* (2007); Sacconi (1954).



Experimental

Crystal data

$$\begin{split} & [\mathrm{Mn}_2(\mathrm{C}_{15}\mathrm{H}_{13}\mathrm{N}_2\mathrm{O}_3)_3]\mathrm{ClO}_4\cdot\mathrm{CH}_4\mathrm{O} \\ & M_r = 1049.19 \\ & \mathrm{Triclinic}, \ P\overline{1} \\ & a = 12.7184 \ (6) \ \text{\AA} \\ & b = 13.8723 \ (7) \ \text{\AA} \\ & c = 15.0885 \ (12) \ \text{\AA} \\ & \alpha = 100.268 \ (1)^\circ \\ & \beta = 94.030 \ (1)^\circ \end{split}$$

Data collection

Bruker APEXII CCD diffractometer Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $T_{min} = 0.906, T_{max} = 0.936$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.045$ $wR(F^2) = 0.123$ S = 1.058138 reflections

Table 1			_
Selected	bond	lengths	(Å).

Mn1-O2	2.099 (2)	Mn2-O1	2.427 (2)
Mn1-O3	2.148 (2)	Mn2-O2	2.083 (2)
Mn1-O8	2.105 (2)	Mn2-O5	2.061 (2)
Mn1-O9	2.196 (2)	Mn2-O6	2.192 (2)
Mn1-N1	2.263 (2)	Mn2-O8	2.215 (2)
Mn1-N5	2.253 (3)	Mn2-N3	2.200 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdot \cdot \cdot A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$N2-H2A\cdots O5^{i}$	0.88	2.04	2.907 (3)	168
$N4-H4A\cdots O13^{ii}$	0.88	2.08	2.910 (4)	156
N6-H6A···O14	0.88	1.98	2.810 (4)	156
$O14-H14A\cdots O10^{iii}$	0.84	2.05	2.865 (4)	165

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2307).

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Bis[#-2-(2-benzoylhydrazinylidenemethyl)-6-methoxyphenolato][2-(2-benzoylhydrazinylidenemethyl)-6-methoxyphenolato]dimanganese(II) perchlorate methanol solvate

G.-M. Yu, Y.-H. Li, L.-F. Zou, J.-W. Zhu and X.-Q. Liu

Comment

Studies of Schiff base compounds are of great interest in various aspects of chemistry, such as homogeneous catalysts in industry, antitumor activities, photoelectric materials, catalytic materials, etc. (Ando *et al.*, 2004; Costes *et al.*, 1995; Duda *et al.*, 2003; Siddall *et al.*, 1983). The crystal structures of metal complexes with salicylaldehyde benzoylhydrazide have been attracted tremendous interest (Huang & Li, 2007; Yin, 2008; Yu *et al.*, 2006). As a continuation of our effort in this system, we investigated a novel Schiff base, 3-methoxysalicylaldehyde benzoylhydrazide (H₂L). This multidentate ligand has several O and N donors with suitable relative positions, which can coordinate to two or more metal centers. In addition, the vanillin group displays a variety of bonding geometries, such as monodentate, chelating, bidentate bridging, monodentate bridging, and chelating bridging (Li *et al.*, 2010). We report here the synthesis and crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. There are two crystallographically independent Mn^{II} centers with different coordination environments in the asymmetric unit. The two Mn^{II} ions, Mnl and Mn2, are bridged by two phenolate O atoms (O2, O8) from two Schiff base ligands (Table 1). The Mn1···Mn2 separation is 3.284 (1) Å, and the Mn1–O2–Mn2 and Mn1–O8–Mn2 angles are 103.50 (9) and 98.92 (8)°, respectively. The coordination geometry of each Mn^{II} ion is distorted octahedral. The Mn1 atom is coordinated by two N atoms and four O atoms from two ligands. The square plane around the Mn1 atom is formed by O_2N_2 donor atoms (N1, N5, O8 and O9) and the axial positions are occupied by phenolate O2 and carbonyl O3. However, the Mn2 atom is coordinated by one N atom and five O atoms from three ligands. The distorted octahedral coordination is achieved by the equatorial plane donor atoms, methoxy O1, carbonyl O2, phenolate O8 and hydrazine N3, and the coordination of phenolate O5 and carbonyl O6 at the axial positions. In addition, the methoxy O1 is weakly bonded to Mn2 with a Mn2–O1 distance of 2.427 (2) Å, which is comparable to those reported for other binuclear Mn^{II} complexes (Mikuriya *et al.*, 1992). In the crystal structure, two adjacent molecules participate in complementary N(hydrazine)–H···O(phenolate) hydrogen bonds, forming a dimeric structure (Fig. 2 and Table 2). The dimers, perchlorate anions and methanol solvent molecules are further connected into a chain structure through N–H···O and O–H···O hydrogen bonds (Fig. 3).

Experimental

The Schiff base ligand (H_2L) was prepared in a similar manner to the reported procedures (Pouralimardan *et al.*, 2007; Sacconi, 1954). The title compound was synthesized by adding Mn(ClO₄)₂.6H₂O (36.6 mg, 0.1 mmol) and imidazole(6.8 mg, 0.1 mmol) to a solution of H_2L (27.3 mg, 0.1 mmol) in methanol (15 ml). The resulting mixture was stirred for 5 h at room temperature to afford a yellow solution, which was left unperturbed to allow slow evaporation of the solvent. Yellow single crystals suitable for X-ray diffraction analysis were formed after about two weeks.

Refinement

H atoms were placed in calculated positions and refined using a riding model, with C-H (aromatic) = 0.95 and 0.98 (methyl) Å, N—H = 0.88 Å and O—H = 0.84 Å and with $U_{iso}(H) = 1.2(1.5 \text{ for methyl and hydroxy})U_{eq}(C, N, O)$.

Figures



Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.



Fig. 2. The dimeric structure of the title compound, with hydrogen bonds shown as green dashed lines.

Fig. 3. One-dimensional chain structure of the title compound. Hydrogen bonds are shown as dashed lines.

Bis[µ-2-(2-benzoylhydrazinylidenemethyl)-6-methoxyphenolato][2-(2-benzoylhydrazinylidenemethyl)-6methoxyphenolato]dimanganese(II) perchlorate methanol solvate

Crystal data

[Mn ₂ (C ₁₅ H ₁₃ N ₂ O ₃) ₃]ClO ₄ ·CH ₄ O	Z = 2
$M_r = 1049.19$	F(000) = 1080
Triclinic, $P\overline{1}$	$D_{\rm x} = 1.499 {\rm Mg m}^{-3}$
Hall symbol: -P 1	Mo K α radiation, $\lambda = 0.71073$ Å
a = 12.7184 (6) Å	Cell parameters from 5673 reflections
b = 13.8723 (7) Å	$\theta = 2.4 - 25.9^{\circ}$
c = 15.0885 (12) Å	$\mu = 0.68 \text{ mm}^{-1}$
$\alpha = 100.268 \ (1)^{\circ}$	T = 173 K
$\beta = 94.030 \ (1)^{\circ}$	Block, yellow
$\gamma = 115.826 (1)^{\circ}$	$0.15\times0.12\times0.10~mm$
V = 2324.7 (2) Å ³	
Data collection	
Bruker APEXII CCD	

diffractometer	8138 independent reflections
Radiation source: fine-focus sealed tube	6183 reflections with $I > 2\sigma(I)$
graphite	$R_{\rm int} = 0.021$

ϕ and ω scans	$\theta_{\text{max}} = 25.0^{\circ}, \ \theta_{\text{min}} = 1.8^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 10$
$T_{\min} = 0.906, \ T_{\max} = 0.936$	$k = -16 \rightarrow 16$
11959 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.045$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.123$	H-atom parameters constrained
<i>S</i> = 1.05	$w = 1/[\sigma^2(F_0^2) + (0.0586P)^2 + 1.186P]$ where $P = (F_0^2 + 2F_c^2)/3$
8138 reflections	$(\Delta/\sigma)_{\rm max} = 0.001$
627 parameters	$\Delta \rho_{max} = 0.49 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta \rho_{min} = -0.68 \text{ e} \text{ Å}^{-3}$

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

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
Cl1	0.89876 (8)	0.67575 (8)	0.50975 (6)	0.0426 (2)
Mn1	0.36982 (4)	0.89528 (4)	0.15072 (3)	0.02431 (13)
Mn2	0.43109 (4)	1.15354 (4)	0.23009 (3)	0.03144 (15)
N1	0.4807 (2)	0.87719 (19)	0.04411 (16)	0.0228 (5)
N2	0.4219 (2)	0.77597 (19)	-0.01720 (16)	0.0251 (6)
H2A	0.4560	0.7548	-0.0600	0.030*
N3	0.3403 (2)	1.2330 (2)	0.31023 (17)	0.0293 (6)
N4	0.3060 (2)	1.1885 (2)	0.38472 (18)	0.0322 (6)
H4A	0.2582	1.2037	0.4174	0.039*
N5	0.2727 (2)	0.8410 (2)	0.26601 (17)	0.0267 (6)
N6	0.3164 (2)	0.7859 (2)	0.31286 (17)	0.0294 (6)
H6A	0.2818	0.7550	0.3559	0.035*
01	0.64422 (19)	1.24458 (18)	0.27865 (15)	0.0357 (5)
O2	0.50670 (18)	1.05637 (16)	0.17192 (15)	0.0293 (5)
O3	0.26225 (19)	0.74323 (17)	0.05223 (14)	0.0308 (5)
O4	0.4299 (2)	1.3273 (2)	0.00081 (16)	0.0468 (7)
O5	0.43845 (19)	1.26231 (17)	0.15090 (14)	0.0312 (5)
06	0.42445 (19)	1.10827 (19)	0.36227 (15)	0.0344 (5)
O7	0.1612 (2)	1.08089 (19)	0.09004 (16)	0.0377 (6)
08	0.27945 (18)	0.99182 (17)	0.16429 (14)	0.0287 (5)
09	0.46239 (19)	0.82750 (19)	0.22884 (15)	0.0337 (5)
O10	1.0073 (2)	0.6796 (2)	0.54667 (19)	0.0528 (7)
011	0.8019 (3)	0.5765 (2)	0.5162 (3)	0.0818 (11)
012	0.9022 (3)	0.6841 (4)	0.4178 (2)	0.0971 (13)
013	0.8851 (3)	0.7656 (2)	0.5595 (2)	0.0648 (8)

O14	0.1488 (2)	0.6610(2)	0.41134 (19)	0.0510(7)
H14A	0.1138	0.6790	0.4513	0.077*
C1	0.7174 (3)	1.3365 (3)	0.3523 (2)	0.0494 (10)
H1A	0.7737	1.3195	0.3857	0.074*
H1B	0.6677	1.3518	0.3938	0.074*
H1C	0.7609	1.4012	0.3280	0.074*
C2	0.6994 (3)	1.2000 (3)	0.2201 (2)	0.0273 (7)
C3	0.8167 (3)	1.2503 (3)	0.2135 (2)	0.0330 (8)
H3	0.8690	1.3194	0.2531	0.040*
C4	0.8587 (3)	1.1981 (3)	0.1472 (2)	0.0378 (8)
H4	0.9399	1.2327	0.1412	0.045*
C5	0.7840 (3)	1.0981 (3)	0.0912 (2)	0.0310(7)
H5	0.8140	1.0643	0.0463	0.037*
C6	0.6630 (3)	1.0438 (2)	0.0988 (2)	0.0243 (7)
C7	0.6198 (3)	1.0971 (2)	0.1639 (2)	0.0238 (7)
C8	0.5897 (3)	0.9368 (2)	0.0389 (2)	0.0244 (7)
H8	0.6239	0.9091	-0.0066	0.029*
C9	0.3099 (3)	0.7115 (3)	-0.0082 (2)	0.0270 (7)
C10	0.2450 (3)	0.6014 (3)	-0.0711 (2)	0.0308 (7)
C11	0.2905 (3)	0.5623 (3)	-0.1418 (2)	0.0351 (8)
H11	0.3678	0.6075	-0.1520	0.042*
C12	0.2250 (4)	0.4588 (3)	-0.1973 (3)	0.0487 (10)
H12	0.2567	0.4338	-0.2463	0.058*
C13	0.1160 (4)	0.3924 (4)	-0.1825 (3)	0.0705 (14)
H13	0.0710	0.3212	-0.2215	0.085*
C14	0.0703 (4)	0.4277 (4)	-0.1116 (4)	0.0882 (19)
H14	-0.0052	0.3801	-0.0999	0.106*
C15	0.1342 (4)	0.5327 (3)	-0.0570 (3)	0.0615 (12)
H15	0.1011	0.5577	-0.0090	0.074*
C16	0.4032 (4)	1.3346 (4)	-0.0898 (3)	0.0576 (11)
H16A	0.3172	1.2961	-0.1099	0.086*
H16B	0.4408	1.3006	-0.1304	0.086*
H16C	0.4331	1.4122	-0.0919	0.086*
C17	0.3771 (3)	1.3615 (3)	0.0659 (2)	0.0399 (9)
C18	0.3230 (4)	1.4265 (3)	0.0576 (3)	0.0507 (10)
H18	0.3211	1.4513	0.0030	0.061*
C19	0.2704 (4)	1.4567 (3)	0.1289 (3)	0.0573 (12)
H19	0.2341	1.5029	0.1235	0.069*
C20	0.2720 (4)	1.4192 (3)	0.2055 (3)	0.0509 (10)
H20	0.2361	1.4398	0.2536	0.061*
C21	0.3251 (3)	1.3508 (3)	0.2163 (2)	0.0349 (8)
C22	0.3833 (3)	1.3234 (3)	0.1464 (2)	0.0325 (8)
C23	0.3085 (3)	1.3055 (3)	0.2952 (2)	0.0357 (8)
H23	0.2713	1.3307	0.3397	0.043*
C24	0.3494 (3)	1.1208 (3)	0.4046 (2)	0.0298 (7)
C25	0.3037 (3)	1.0616 (3)	0.4763 (2)	0.0309 (7)
C26	0.1919 (3)	1.0360 (3)	0.4984 (2)	0.0372 (8)
H26	0.1430	1.0614	0.4700	0.045*
C27	0.1522 (3)	0.9736 (3)	0.5616 (2)	0.0459 (9)

H27	0.0747	0.9540	0.5752	0.055*
C28	0.2237 (4)	0.9395 (3)	0.6051 (3)	0.0506 (10)
H28	0.1958	0.8977	0.6495	0.061*
C29	0.3351 (4)	0.9651 (3)	0.5852 (3)	0.0496 (10)
H29	0.3848	0.9421	0.6159	0.060*
C30	0.3739 (3)	1.0248 (3)	0.5200 (3)	0.0436 (9)
H30	0.4500	1.0410	0.5047	0.052*
C31	0.1054 (3)	1.1402 (3)	0.0565 (3)	0.0461 (9)
H31A	0.0234	1.0889	0.0279	0.069*
H31B	0.1486	1.1769	0.0112	0.069*
H31C	0.1059	1.1954	0.1073	0.069*
C32	0.1105 (3)	1.0228 (3)	0.1532 (2)	0.0317 (8)
C33	0.0058 (3)	1.0108 (3)	0.1813 (2)	0.0404 (9)
H33	-0.0358	1.0457	0.1574	0.049*
C34	-0.0395 (3)	0.9480 (3)	0.2444 (2)	0.0413 (9)
H34	-0.1120	0.9400	0.2633	0.050*
C35	0.0195 (3)	0.8980 (3)	0.2794 (2)	0.0352 (8)
H35	-0.0121	0.8558	0.3229	0.042*
C36	0.1272 (3)	0.9079 (3)	0.2519 (2)	0.0284 (7)
C37	0.1759 (3)	0.9730 (3)	0.1888 (2)	0.0273 (7)
C38	0.1829 (3)	0.8511 (2)	0.2921 (2)	0.0282 (7)
H38	0.1513	0.8191	0.3408	0.034*
C39	0.4151 (3)	0.7819 (3)	0.2892 (2)	0.0295 (7)
C40	0.4667 (3)	0.7237 (3)	0.3367 (2)	0.0304 (7)
C41	0.4082 (3)	0.6553 (3)	0.3924 (3)	0.0431 (9)
H41	0.3318	0.6451	0.4031	0.052*
C42	0.4614 (3)	0.6021 (3)	0.4321 (3)	0.0507 (10)
H42	0.4210	0.5548	0.4700	0.061*
C43	0.5727 (4)	0.6170 (3)	0.4175 (3)	0.0477 (10)
H43	0.6080	0.5789	0.4443	0.057*
C44	0.6327 (3)	0.6870 (3)	0.3641 (2)	0.0416 (9)
H44	0.7101	0.6986	0.3550	0.050*
C45	0.5795 (3)	0.7404 (3)	0.3238 (2)	0.0342 (8)
H45	0.6207	0.7888	0.2870	0.041*
C46	0.0717 (4)	0.5557 (4)	0.3563 (4)	0.0767 (15)
H46A	0.1038	0.5429	0.3007	0.115*
H46B	-0.0064	0.5515	0.3398	0.115*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0341 (5)	0.0521 (6)	0.0478 (5)	0.0259 (4)	0.0126 (4)	0.0075 (4)
Mn1	0.0245 (3)	0.0270 (3)	0.0250 (3)	0.0148 (2)	0.0078 (2)	0.00504 (19)
Mn2	0.0328 (3)	0.0336 (3)	0.0319 (3)	0.0191 (2)	0.0108 (2)	0.0045 (2)
N1	0.0270 (14)	0.0203 (13)	0.0225 (13)	0.0124 (11)	0.0055 (11)	0.0036 (10)
N2	0.0286 (15)	0.0252 (14)	0.0216 (13)	0.0137 (12)	0.0065 (11)	0.0013 (11)
N3	0.0305 (15)	0.0319 (15)	0.0262 (14)	0.0150 (12)	0.0094 (12)	0.0046 (12)

N4	0.0356 (16)	0.0368 (16)	0.0322 (15)	0.0218 (13)	0.0167 (13)	0.0086 (12)
N5	0.0258 (14)	0.0299 (14)	0.0271 (14)	0.0159 (12)	0.0062 (11)	0.0043 (11)
N6	0.0303 (15)	0.0369 (16)	0.0291 (14)	0.0194 (13)	0.0112 (12)	0.0136 (12)
01	0.0300 (13)	0.0326 (13)	0.0369 (13)	0.0115 (10)	0.0088 (10)	-0.0036 (10)
O2	0.0227 (12)	0.0262 (12)	0.0380 (13)	0.0121 (10)	0.0108 (10)	0.0002 (10)
O3	0.0291 (12)	0.0310 (12)	0.0310 (12)	0.0140 (10)	0.0096 (10)	0.0015 (10)
O4	0.0661 (18)	0.0687 (18)	0.0340 (13)	0.0499 (16)	0.0220 (13)	0.0228 (13)
O5	0.0357 (13)	0.0332 (12)	0.0311 (12)	0.0197 (11)	0.0111 (10)	0.0095 (10)
O6	0.0314 (13)	0.0426 (14)	0.0345 (13)	0.0213 (11)	0.0101 (10)	0.0082 (11)
O7	0.0361 (13)	0.0443 (14)	0.0446 (14)	0.0265 (12)	0.0085 (11)	0.0157 (12)
O8	0.0234 (11)	0.0343 (12)	0.0337 (12)	0.0171 (10)	0.0087 (10)	0.0084 (10)
09	0.0299 (13)	0.0480 (14)	0.0355 (13)	0.0237 (11)	0.0135 (10)	0.0205 (11)
O10	0.0397 (15)	0.0699 (19)	0.0589 (17)	0.0322 (14)	0.0091 (13)	0.0198 (15)
O11	0.0371 (17)	0.0475 (18)	0.150 (3)	0.0131 (14)	0.0151 (19)	0.014 (2)
O12	0.098 (3)	0.190 (4)	0.0464 (19)	0.100 (3)	0.0219 (18)	0.033 (2)
O13	0.0533 (18)	0.0531 (17)	0.095 (2)	0.0311 (15)	0.0346 (17)	0.0086 (16)
O14	0.0425 (15)	0.0571 (18)	0.0637 (18)	0.0250 (14)	0.0296 (14)	0.0238 (14)
C1	0.048 (2)	0.051 (2)	0.036 (2)	0.019 (2)	0.0038 (18)	-0.0115 (18)
C2	0.0303 (18)	0.0305 (17)	0.0271 (16)	0.0190 (15)	0.0068 (14)	0.0070 (14)
C3	0.0256 (18)	0.0294 (18)	0.0377 (19)	0.0100 (15)	-0.0008 (15)	0.0016 (15)
C4	0.0227 (18)	0.042 (2)	0.049 (2)	0.0153 (16)	0.0102 (16)	0.0070 (17)
C5	0.0264 (18)	0.0385 (19)	0.0347 (18)	0.0210 (16)	0.0093 (14)	0.0063 (15)
C6	0.0265 (17)	0.0291 (17)	0.0238 (16)	0.0173 (14)	0.0069 (13)	0.0082 (13)
C7	0.0214 (16)	0.0285 (17)	0.0248 (16)	0.0138 (14)	0.0050 (13)	0.0073 (13)
C8	0.0275 (17)	0.0295 (17)	0.0234 (16)	0.0189 (14)	0.0084 (13)	0.0065 (13)
С9	0.0298 (18)	0.0278 (17)	0.0268 (17)	0.0163 (15)	0.0053 (14)	0.0064 (13)
C10	0.0296 (18)	0.0285 (17)	0.0333 (18)	0.0132 (15)	0.0053 (14)	0.0047 (14)
C11	0.036 (2)	0.0324 (19)	0.0339 (19)	0.0155 (16)	0.0062 (15)	0.0014 (15)
C12	0.051 (2)	0.040 (2)	0.049 (2)	0.021 (2)	0.0105 (19)	-0.0056 (18)
C13	0.057 (3)	0.041 (2)	0.079 (3)	0.004 (2)	0.014 (2)	-0.019 (2)
C14	0.055 (3)	0.052 (3)	0.104 (4)	-0.010 (2)	0.031 (3)	-0.024 (3)
C15	0.046 (2)	0.043 (2)	0.070 (3)	0.005 (2)	0.023 (2)	-0.012 (2)
C16	0.076 (3)	0.079 (3)	0.040 (2)	0.050 (3)	0.019 (2)	0.021 (2)
C17	0.046 (2)	0.046 (2)	0.040 (2)	0.0293 (19)	0.0168 (17)	0.0145 (17)
C18	0.072 (3)	0.058 (3)	0.047 (2)	0.046 (2)	0.021 (2)	0.024 (2)
C19	0.086 (3)	0.060 (3)	0.059 (3)	0.059 (3)	0.023 (2)	0.022 (2)
C20	0.073 (3)	0.053 (2)	0.048 (2)	0.045 (2)	0.022 (2)	0.0129 (19)
C21	0.040 (2)	0.0361 (19)	0.0350 (19)	0.0234 (17)	0.0111 (16)	0.0069 (15)
C22	0.0320 (19)	0.0300 (18)	0.0377 (19)	0.0164 (15)	0.0082 (15)	0.0065 (15)
C23	0.041 (2)	0.0362 (19)	0.0359 (19)	0.0247 (17)	0.0124 (16)	0.0029 (15)
C24	0.0245 (17)	0.0315 (18)	0.0279 (17)	0.0111 (14)	0.0031 (14)	-0.0010 (14)
C25	0.0309 (18)	0.0310 (18)	0.0292 (17)	0.0134 (15)	0.0093 (14)	0.0035 (14)
C26	0.034 (2)	0.042 (2)	0.0322 (18)	0.0165 (17)	0.0067 (15)	0.0046 (16)
C27	0.036 (2)	0.052 (2)	0.041 (2)	0.0116 (18)	0.0108 (17)	0.0122 (18)
C28	0.061 (3)	0.046 (2)	0.046 (2)	0.021 (2)	0.017 (2)	0.0185 (19)
C29	0.057 (3)	0.053 (2)	0.052 (2)	0.033 (2)	0.011 (2)	0.022 (2)
C30	0.044 (2)	0.050 (2)	0.046 (2)	0.0287 (19)	0.0134 (18)	0.0125 (18)
C31	0.042 (2)	0.043 (2)	0.062 (3)	0.0269 (19)	0.0021 (19)	0.0165 (19)
C32	0.0263 (18)	0.0353 (19)	0.0351 (18)	0.0183 (15)	0.0033 (15)	0.0013 (15)

C33	0.034 (2)	0.056 (2)	0.042 (2)	0.0321 (19)	0.0059 (16)	0.0061 (18)
C34	0.0263 (19)	0.055 (2)	0.045 (2)	0.0235 (18)	0.0099 (16)	0.0029 (18)
C35	0.0274 (18)	0.0365 (19)	0.0384 (19)	0.0139 (16)	0.0096 (15)	0.0014 (15)
C36	0.0223 (16)	0.0312 (17)	0.0291 (17)	0.0137 (14)	0.0036 (13)	-0.0026 (14)
C37	0.0229 (17)	0.0287 (17)	0.0276 (17)	0.0138 (14)	0.0021 (13)	-0.0045 (13)
C38	0.0241 (17)	0.0288 (17)	0.0287 (17)	0.0109 (14)	0.0077 (14)	0.0015 (14)
C39	0.0311 (18)	0.0306 (17)	0.0274 (17)	0.0149 (15)	0.0054 (14)	0.0063 (14)
C40	0.0318 (18)	0.0296 (17)	0.0315 (18)	0.0159 (15)	0.0055 (14)	0.0065 (14)
C41	0.036 (2)	0.049 (2)	0.049 (2)	0.0191 (18)	0.0078 (17)	0.0239 (19)
C42	0.042 (2)	0.053 (2)	0.060 (3)	0.019 (2)	0.0020 (19)	0.030 (2)
C43	0.059 (3)	0.043 (2)	0.050 (2)	0.032 (2)	-0.003 (2)	0.0135 (19)
C44	0.045 (2)	0.051 (2)	0.038 (2)	0.0332 (19)	-0.0008 (17)	0.0027 (17)
C45	0.040 (2)	0.041 (2)	0.0289 (18)	0.0257 (17)	0.0073 (15)	0.0061 (15)
C46	0.054 (3)	0.058 (3)	0.120 (4)	0.028 (3)	0.023 (3)	0.016 (3)

Geometric parameters (Å, °)

Cl1—O12	1.414 (3)	C12—C13	1.351 (6)
Cl1-011	1.418 (3)	C12—H12	0.9500
Cl1—O13	1.422 (3)	C13—C14	1.368 (6)
Cl1—O10	1.428 (3)	C13—H13	0.9500
Mn1—O2	2.099 (2)	C14—C15	1.381 (6)
Mn1—O3	2.148 (2)	C14—H14	0.9500
Mn1—08	2.105 (2)	C15—H15	0.9500
Mn1—09	2.196 (2)	C16—H16A	0.9800
Mn1—N1	2.263 (2)	C16—H16B	0.9800
Mn1—N5	2.253 (3)	C16—H16C	0.9800
Mn2—O1	2.427 (2)	C17—C18	1.367 (5)
Mn2—O2	2.083 (2)	C17—C22	1.419 (5)
Mn2—O5	2.061 (2)	C18—C19	1.403 (5)
Mn2—O6	2.192 (2)	C18—H18	0.9500
Mn2—O8	2.215 (2)	C19—C20	1.351 (5)
Mn2—N3	2.200 (3)	C19—H19	0.9500
Mn1—Mn2	3.284 (1)	C20—C21	1.407 (5)
N1—C8	1.285 (4)	C20—H20	0.9500
N1—N2	1.383 (3)	C21—C22	1.420 (4)
N2—C9	1.344 (4)	C21—C23	1.430 (5)
N2—H2A	0.8800	C23—H23	0.9500
N3—C23	1.284 (4)	C24—C25	1.473 (4)
N3—N4	1.384 (4)	C25—C26	1.388 (5)
N4	1.343 (4)	C25—C30	1.388 (5)
N4—H4A	0.8800	C26—C27	1.376 (5)
N5—C38	1.289 (4)	C26—H26	0.9500
N5—N6	1.377 (3)	C27—C28	1.372 (5)
N6—C39	1.350 (4)	C27—H27	0.9500
N6—H6A	0.8800	C28—C29	1.372 (6)
O1—C2	1.388 (4)	C28—H28	0.9500
01—C1	1.429 (4)	C29—C30	1.378 (5)
O2—C7	1.320 (3)	C29—H29	0.9500

04-C17 1358 (4) $C31-H31A$ $0,9800$ $04-C16$ 1.418 (4) $C31-H31B$ $0,9800$ $05-C22$ 1.322 (4) $C31-H31C$ $0,9800$ $05-C22$ 1.372 (4) $C32-C33$ 1.375 (4) $07-C31$ 1.430 (4) $C33-C34$ 1.391 (5) $07-C31$ 1.320 (4) $C34-C35$ 1.561 (5) $014-C46$ 1.410 (5) $C34-H34$ 0.9500 $014-C46$ 1.410 (5) $C34-H34$ 0.9500 $014-C46$ 1.410 (5) $C34-H34$ 0.9500 $014-C46$ 1.410 (5) $C34-C37$ 1.417 (5) $014-C16$ 0.9800 $C35-C36$ 1.445 (4) $C2-C3$ 1.364 (4) $C38-H38$ 0.9500 $C1-H1B$ 0.9800 $C36-C37$ 1.435 (5) $C-C7$ 1.404 (4) $C39-C40$ 1.485 (4) $C3-C4$ 1.401 (5) $C40-C41$ 1.385 (5) $C4-C5$ 1.365 (5) $C41-C42$ 0.9500 $C4-C4$ 1.380 (5) $C4-C43$ 1.380 (5)	О3—С9	1.249 (4)	С30—Н30	0.9500
04-C16 1.418 (4) $C31-H31B$ 0.9800 $05-C22$ 1.322 (4) $C32-C33$ 1.375 (4) $07-C32$ 1.372 (4) $C32-C37$ 1.424 (4) $07-C32$ 1.372 (4) $C32-C37$ 1.424 (4) $07-C32$ 1.372 (4) $C33-H33$ 0.9500 $09-C39$ 1.242 (4) $C34-H33$ 0.9500 $014-C166$ 1.410 (5) $C34-H34$ 0.9500 $014-C166$ 0.9800 $C35-C35$ 1.416 (4) $C1-H1A$ 0.9800 $C36-C37$ 1.445 (4) $C2-C7$ 1.404 (4) $C39-C40$ 1.483 (4) $C2-C7$ 1.404 (4) $C39-C40$ 1.483 (5) $C4-L4$ 1.401 (5) $C40-C45$ 1.383 (5) $C4-L5$ 1.385 (5) $C41-C42$ 1.390 (5) $C4-L4$ 0.9500 $C42-H42$ 0.9500 $C4-L44$ 0.9500 $C42-H42$ 0.9500 $C5-C6$ 1.410 (4) $C43-H45$ 0.9500 <td>O4—C17</td> <td>1.358 (4)</td> <td>C31—H31A</td> <td>0.9800</td>	O4—C17	1.358 (4)	C31—H31A	0.9800
05-C22 $1322 (4)$ $C31-H31C$ $0,9800$ $06-C24$ $1242 (4)$ $C32-C33$ $1375 (4)$ $07-C32$ $1372 (4)$ $C32-C37$ $1424 (4)$ $07-C31$ $1430 (4)$ $C33-C34$ $1391 (5)$ $08-C39$ $1242 (4)$ $C34-C35$ $154 (5)$ $00-C39$ $1242 (4)$ $C34-H34$ 0.9500 $014-C46$ $1410 (5)$ $C34-H34$ 0.9500 $014-H1AA$ 0.9800 $C35-C35$ $1414 (4)$ $C2-C3$ $1364 (4)$ $C38-H38$ 0.9500 $C1-H1B$ 0.9800 $C36-C37$ $1417 (5)$ $C1-H1C$ 0.9800 $C36-C38$ $144 (4)$ $C3-C3$ $1364 (4)$ $C38-H38$ 0.9500 $C2-C7$ $1404 (4)$ $C39-C40$ $1483 (4)$ $C3-H3$ 0.9500 $C40-C41$ $1385 (5)$ $C4-C5$ $1365 (5)$ $C41-C42$ $1377 (5)$ $C4-H4$ 0.9500 $C42-C43$ $1380 (5)$ $C5-C6$ $142 (4)$ $C43-H34$ 0.9500 C	O4—C16	1.418 (4)	C31—H31B	0.9800
06-C24 $1242 (4)$ $C32-C33$ $1375 (4)$ $07-C32$ $1372 (4)$ $C32-C37$ $1424 (4)$ $07-C31$ $1430 (4)$ $C33-C34$ $1391 (5)$ $08-C37$ $1220 (4)$ $C33-H33$ 0.9500 $09-C39$ $1242 (4)$ $C34-C35$ $1.361 (5)$ $014-C46$ $1.410 (5)$ $C34-H54$ 0.9500 $01-H1A$ 0.9800 $C35-C36$ $1.416 (4)$ $C1-H1B$ 0.9800 $C36-C37$ $1.417 (5)$ $C1-H1B$ 0.9800 $C36-C38$ $1.445 (4)$ $C2-C7$ $1.404 (4)$ $C39-C40$ $1.483 (4)$ $C3-C4$ $1.401 (5)$ $C40-C45$ $1.383 (5)$ $C4-C5$ $1.365 (5)$ $C41-C42$ $1.377 (5)$ $C4-C5$ $1.360 (5)$ $C4-H44$ 0.9500 $C5-C6$ $1.412 (4)$ $C43-C43$ $1.380 (5)$ $C5-C6$ $1.444 (4)$ $C43-H43$ 0.9500 $C6-C7$ $1.410 (4)$ $C43-H43$ 0.9500 $C5-C6$ $1.424 (5)$ $C46-H46A$ 0.9800	O5—C22	1.322 (4)	C31—H31C	0.9800
07-C32 $1.372 (4)$ $C32-C37$ $1.424 (4)$ $07-C31$ $1.430 (4)$ $C33-C34$ $1.391 (5)$ $08-C37$ $1.320 (4)$ $C33-C34$ $1.391 (5)$ $09-C39$ $1.242 (4)$ $C34-C35$ $1.361 (5)$ $014-C46$ $1.410 (5)$ $C34-H34$ 0.9500 $014-H1A$ 0.9800 $C35-C36$ $1.416 (4)$ $C1-H1A$ 0.9800 $C36-C37$ $1.417 (5)$ $C1-H1B$ 0.9800 $C36-C37$ $1.4147 (5)$ $C2-C3$ $1.364 (4)$ $C38-H38$ 0.9500 $C2-C7$ $1.404 (4)$ $C39-C40$ $1.483 (4)$ $C2-C3$ $1.364 (4)$ $C39-C40$ $1.483 (5)$ $C3-C4$ $1.401 (5)$ $C40-C45$ $1.383 (5)$ $C3-C4$ $1.401 (5)$ $C40-C45$ $1.383 (5)$ $C4-C5$ $1.365 (5)$ $C41-C42$ $1.377 (5)$ $C4-C4$ $1.401 (5)$ $C42-C43$ $1.380 (5)$ $C5-C6$ $1.412 (4)$ $C42-C43$ $1.380 (5)$ $C5-C6$ $1.412 (4)$ $C42-H42$ 0.9500 $C6-C7$ $1.410 (4)$ $C43-H43$ 0.9500 $C6-C8$ $1.444 (4)$ $C43-H43$ 0.9500 $C1-C10$ $1.480 (4)$ $C44-H44$ 0.9500 $C1-C11$ $1.35 (4)$ $C46-H46A$ 0.9800 $C11-C12$ $1.374 (5)$ $C46-H46A$ 0.9800 $C1-C11$ $1.35 (4)$ $C45-H45$ 0.9500 $C1-C11$ $1.98 (4)$ $C13-C14-H14$ 120.0 $O12-C11-O13$ $108 5(18)$ $C13-C14-H14$ </td <td>O6—C24</td> <td>1.242 (4)</td> <td>C32—C33</td> <td>1.375 (4)</td>	O6—C24	1.242 (4)	C32—C33	1.375 (4)
07-C31 1430 (4) $C33-C34$ 1391 (5) $08-C37$ 1320 (4) $C33-H133$ 0.9500 $09-C39$ 1224 (4) $C34-C155$ 1361 (5) $014-C46$ 1410 (5) $C34-H34$ 0.9500 $014-H14A$ 0.9800 $C35-C36$ 1.416 (4) $C1-H1B$ 0.9800 $C36-C37$ 1.417 (5) $C1-H1B$ 0.9800 $C36-C38$ 1.445 (4) $C2-C3$ 1.364 (4) $C38-H38$ 0.9500 $C2-C7$ 1.404 (4) $C39-C40$ 1.483 (4) $C2-C7$ 1.404 (4) $C39-C40$ 1.483 (5) $C3-H3$ 0.9500 $C40-C45$ 1.385 (5) $C3-H3$ 0.9500 $C40-C45$ 1.385 (5) $C4-C5$ 1.365 (5) $C41-C42$ 1.377 (5) $C4-H4$ 0.9500 $C42-H42$ 0.9500 $C5-C6$ 1.412 (4) $C43-C44$ 1.386 (5) $C5-H5$ 0.9500 $C42-H42$ 0.9500 $C5-C6$ 1.444 (4) $C43-H43$ 0.9500 $C6-C7$ 1.410 (4) $C43-H43$ 0.9500 $C6-C7$ 1.410 (4) $C43-H43$ 0.9500 $C6-C8$ 1.444 (4) $C43-H43$ 0.9500 $C10-C15$ 1.373 (5) $C4-H45$ 0.9800 $C11-C12$ 1.374 (5) $C46-H46A$ 0.9800 $C11-C12$ 1.374 (5) $C16-H16B$ 0.9800 $C11-C11-O13$ 108.39 (19) $C13-C14-C15$ 119.8 (4) $O12-C11-O11$ 112.35 (16) $C14-C15-H15$ 11	O7—C32	1.372 (4)	C32—C37	1.424 (4)
08-C37 1320 (4) $C33-H33$ 0.9500 $09-C39$ 1242 (4) $C34-C35$ 1.361 (5) $014-C46$ 1410 (5) $C34-H34$ 0.9500 $014-H14A$ 0.8400 $C35-C36$ 1.416 (4) $C1-H1B$ 0.9800 $C36-C37$ 1.417 (5) $C1-H1B$ 0.9800 $C36-C38$ 1.445 (4) $C2-C7$ 1.404 (4) $C39-C40$ 1.438 (4) $C3-C4$ 1.401 (5) $C40-C45$ 1.338 (5) $C3-C4$ 1.401 (5) $C40-C45$ 1.338 (5) $C3-C4$ 1.401 (5) $C40-C45$ 1.338 (5) $C3-C4$ 1.401 (5) $C4-C45$ 1.338 (5) $C3-C5$ 1.365 (5) $C41-C42$ 1.377 (5) $C4-C5$ 1.412 (4) $C42-H42$ 0.9500 $C5-C6$ 1.412 (4) $C42-H43$ 1.376 (5) $C6-C7$ 1.440 (4) $C43-H44$ 0.9500 $C6-C7$ 1.440 (4) $C43-H45$ 0.9500 $C10-C15$ 1.373 (5) $C44-H46$ 0.9500 </td <td>O7—C31</td> <td>1.430 (4)</td> <td>C33—C34</td> <td>1.391 (5)</td>	O7—C31	1.430 (4)	C33—C34	1.391 (5)
09-C391242 (4)C34-C351.361 (5)014-C461.410 (5)C34-H340.9500014-H1AA0.9800C35-H350.9500C1-H1A0.9800C36-C371.417 (5)C1-H1B0.9800C36-C381.445 (4)C2-C31.364 (4)C39-C401.483 (4)C2-C71.404 (4)C39-C401.483 (5)C2-C31.364 (7)C40-C411.385 (5)C4-C51.365 (5)C41-C421.377 (5)C4-C51.365 (5)C41-C421.378 (5)C5-C61.412 (4)C42-C431.380 (5)C5-C61.412 (4)C42-C431.380 (5)C5-C61.412 (4)C42-C431.380 (5)C5-C61.412 (4)C42-C431.380 (5)C6-C71.410 (4)C43-H420.9500C6-C71.410 (4)C43-H430.9500C6-C71.410 (4)C43-H430.9500C6-C71.410 (4)C43-H440.9500C10-C151.373 (5)C46-H46A0.9800C10-C111.335 (4)C46-H46A0.9800C10-C111.335 (4)C46-H46B0.9800C11-C121.374 (5)C13-C14-C15119.6C12-C11-O13108.72C14-C15-H15119.6C12-C11-O13108.730C13-C14-H14120.1O11-C11-O10109.91 (18)C13-C14-H14120.1O11-C11-O10109.91 (18)C13-C14-H14120.1O11-C11-O13108.72C14-C15-H15119.6	O8—C37	1.320 (4)	С33—Н33	0.9500
014C46 1.410 (5) C34H34 0.9500 014H114A 0.8400 C35C36 1.416 (4) C1H11A 0.9800 C36C37 1.417 (5) C1H11B 0.9800 C36C37 1.417 (5) C1H11C 0.9800 C36C37 1.435 (4) C2C3 1.364 (4) C39C40 1.438 (4) C3C4 1.401 (5) C40C45 1.383 (5) C3C4 1.401 (5) C40C41 1.385 (5) C4C5 1.365 (5) C41C42 1.377 (5) C4H4 0.9500 C41H41 0.9500 C5C6 1.412 (4) C42C43 1.380 (5) C5C6 1.410 (4) C43H43 0.9500 C6C7 1.410 (4) C43H43 0.9500 C6C7 1.410 (4) C43H43 0.9500 C10C15 1.373 (5) C46H46A 0.9800 C10C15 1.373 (5) C46H46A 0.9800 C11H11 0.9500 C46H46A	O9—C39	1.242 (4)	C34—C35	1.361 (5)
014-H14A 0.8400 $C35-C36$ $1.416 (4)$ $C1-H1A$ 0.9800 $C35-H25$ 0.9500 $C1-H1B$ 0.9800 $C36-C37$ $1.417 (5)$ $C1-H1C$ 0.9800 $C36-C38$ $1.445 (4)$ $C2-C3$ $1.364 (4)$ $C38-H138$ 0.9500 $C2-C7$ $1.404 (4)$ $C39-C40$ $1.483 (4)$ $C3-C4$ $1.401 (5)$ $C40-C45$ $1.383 (5)$ $C3-H3$ 0.9500 $C40-C41$ $1.385 (5)$ $C4-H4$ 0.9500 $C40-C41$ 0.9500 $C5-C6$ $1.412 (4)$ $C42-C43$ $1.380 (5)$ $C5-C6$ $1.412 (4)$ $C42-C43$ $1.380 (5)$ $C5-C6$ $1.412 (4)$ $C43-C44$ 0.9500 $C6-C7$ $1.410 (4)$ $C43-C44$ 0.9500 $C6-C8$ $1.444 (4)$ $C43-C44$ 0.9500 $C8-H8$ 0.9500 $C44-H45$ 0.9500 $C10-C15$ $1.373 (5)$ $C45-H45$ 0.9500 $C10-C15$ $1.373 (5)$ $C45-H468$ 0.9800 $C11-C12$ $1.374 (5)$ $C46-H468$ 0.9800 $C12-C11-O11$ $11.2 (3)$ $C12-C13-H13$ 120.0 $O12-C11-O13$ 108.72 $C14-C14-H14$ 120.1 $O12-C11-O13$ $108.93 (19)$ $C13-C14-H14$ 120.1 $O12-C11-O10$ $108.54 (18)$ $C13-C14-H14$ 120.1 $O12-C11-O10$ $108.54 (18)$ $C13-C14-H14$ 120.1 $O1-C1-O10$ $108.54 (18)$ $C13-C14-H14$ 120.1 $O2-Mn1-O3$ $45.50 (8)$ <td>O14—C46</td> <td>1.410 (5)</td> <td>C34—H34</td> <td>0.9500</td>	O14—C46	1.410 (5)	C34—H34	0.9500
C1—H1A 0.9800 C35—H35 0.9500 C1—H1B 0.9800 C36—C37 1.417 (5) C1—H1C 0.9800 C36—C38 1.445 (4) C2—C3 1.364 (4) C38—H38 0.9500 C2—C7 1.404 (4) C39—C40 1.483 (4) C3—H3 0.9500 C40—C45 1.383 (5) C3—H3 0.9500 C41—C42 1.377 (5) C4—C5 1.365 (5) C41—C42 1.380 (5) C5—C6 1.412 (4) C42—C43 1.380 (5) C5—H5 0.9500 C42—H42 0.9500 C6—C7 1.410 (4) C43—C44 1.376 (5) C6—C8 1.444 (4) C43—H43 0.9500 C8—H8 0.9500 C44—C45 1.384 (5) C9—C10 1.480 (4) C46—H46A 0.9800 C11—C12 1.373 (5) C45—H45 0.9800 C11—C11 1.388 (4) C46—H46A 0.9800 C11—C12 1.374 (5) C46—H46A 0.9800 <t< td=""><td>O14—H14A</td><td>0.8400</td><td>C35—C36</td><td>1.416 (4)</td></t<>	O14—H14A	0.8400	C35—C36	1.416 (4)
C1—H1B 0.9800 C36—C37 1.417 (5) C1—H1C 0.9800 C36—C38 1.445 (4) C2—C3 1.364 (4) C38—H38 0.9500 C2—C7 1.404 (4) C39—C40 1.483 (4) C3—C4 1.401 (5) C40—C45 1.383 (5) C3—H3 0.9500 C41—C42 1.377 (5) C4—C4 0.9500 C41—H41 0.9500 C5—C6 1.412 (4) C42—C43 1.380 (5) C5—H5 0.9500 C44—H42 0.9500 C6—C7 1.410 (4) C43—C44 1.376 (5) C6—C8 1.444 (4) C43—C44 0.9500 C10—C15 1.373 (5) C46—H44 0.9500 C10—C15 1.373 (5) C45—H44 0.9500 C10—C15 1.374 (5) C46—H46A 0.9800 C11—C12 1.374 (5) C46—H46C 0.9800 C12—C11—O13 108.7 (2) C14—C13—H13 120.0 O12—C11—O13 108.39 (19) C13—C14—C15 119.8 (4) </td <td>C1—H1A</td> <td>0.9800</td> <td>С35—Н35</td> <td>0.9500</td>	C1—H1A	0.9800	С35—Н35	0.9500
C1-H1C0.9800C36-C381.445 (4)C2-C31.364 (4)C38-H380.9500C2-C71.404 (4)C39-C401.483 (4)C3-C41.401 (5)C40-C451.383 (5)C3-H30.9500C40-C411.385 (5)C4-C51.365 (5)C41-C421.377 (5)C4-H40.9500C41-H110.9500C5-C61.412 (4)C42-C431.380 (5)C5-C61.412 (4)C42-C430.9500C6-C71.410 (4)C43-C440.9500C6-C71.414 (4)C43-H430.9500C6-C81.373 (5)C45-H450.9500C10-C151.373 (5)C45-H450.9500C10-C111.385 (4)C46-H46A0.9800C11-C121.374 (5)C46-H46A0.9800C11-C111.112 (3)C12-C13-H13120.0C11-C111.182 (4)C13-C14-C15119.6C12-C11-O13108.39 (19)C13-C14-C15119.6C12-C11-O13108.39 (19)C13-C14-H14120.1C11-C11-O10109.91 (18)C15-C14-H14120.1C11-C11-O10109.91 (18)C15-C14-H14120.1C11-C11-O10109.91 (18)C15-C14-H14120.1C11-C11-O10109.91 (18)C15-C14-H14120.1C11-C11-O10109.91 (18)C15-C14-H16B109.5C3-Mn1-O876.87 (8)C10-C15-H15119.6C2-Mn1-O3145.50 (8)C14-C15-H16B109.5C3-Mn1-O998.66 (9) <td< td=""><td>C1—H1B</td><td>0.9800</td><td>C36—C37</td><td>1.417 (5)</td></td<>	C1—H1B	0.9800	C36—C37	1.417 (5)
C2-C31.364 (4) $C38-H38$ 0.9500 $C2-C7$ 1.404 (4) $C39-C40$ 1.483 (4) $C3-C4$ 1.401 (5) $C40-C45$ 1.383 (5) $C3-H3$ 0.9500 $C40-C41$ 1.385 (5) $C4-C5$ 1.365 (5) $C41-C42$ 1.377 (5) $C4-H4$ 0.9500 $C41-H41$ 0.9500 $C5-C6$ 1.412 (4) $C42-C43$ 1.380 (5) $C5-C6$ 1.410 (4) $C43-C44$ 1.376 (5) $C6-C7$ 1.410 (4) $C43-C44$ 1.376 (5) $C6-C8$ 1.444 (4) $C43-H43$ 0.9500 $C8-H8$ 0.9500 $C44-C45$ 1.384 (5) $C9-C10$ 1.480 (4) $C44-H44$ 0.9500 $C10-C15$ 1.373 (5) $C45-H45$ 0.9500 $C10-C11$ 1.385 (4) $C46-H46R$ 0.9800 $C11-C11$ 1.385 (4) $C46-H46R$ 0.9800 $C11-C12$ 1.374 (5) $C46-H46R$ 0.9800 $C11-C11$ 1.283 (4) $C12-C13-H13$ 120.0 $O12-C11-O11$ 108.7 (2) $C14-C13-H13$ 120.0 $O12-C11-O11$ 108.7 (2) $C14-C15-H15$ 119.8 (4) $O12-C11-O11$ 108.54 (18) $C13-C14-H14$ 120.1 $O11-C11-O10$ 109.91 (18) $C13-C14-H14$ 120.1 $O11-C11-O10$ 109.91 (8) $C14-C15-H15$ 119.6 $O2-Mn1-O3$ 145.50 (8) $C14-C15-H15$ 119.6 $O2-Mn1-O3$ 19.51 (8) $O4-C16-H16R$ 109.5 $O2-Mn1-O3$ 19.52 (9) $O4-C16-H16R$ 109.5 $O2-Mn1-O3$ <td< td=""><td>C1—H1C</td><td>0.9800</td><td>C36—C38</td><td>1.445 (4)</td></td<>	C1—H1C	0.9800	C36—C38	1.445 (4)
C2-C71.404 (4)C39-C401.483 (4)C3-C41.401 (5)C40-C451.383 (5)C3-H30.9500C40-C411.385 (5)C4-C51.366 (5)C41-C421.377 (5)C4-H40.9500C41-H410.9500C5-C61.412 (4)C42-C431.380 (5)C5-H50.9500C42-H420.9500C6-C71.410 (4)C43-C441.376 (5)C6-C81.444 (4)C43-C440.9500C8-H80.9500C44-C451.384 (5)C9-C101.480 (4)C44-H440.9500C10-C151.373 (5)C45-H450.9500C10-C111.385 (4)C46-H46A0.9800C11-C121.374 (5)C46-H46B0.9800C11-C111.12 (3)C12-C13-H13120.0O12-C11-O11111.2 (3)C12-C13-H13120.0O12-C11-O13108.7 (2)C14-C15119.8 (4)O12-C11-O10108.39 (19)C13-C14-C15119.8 (4)O12-C11-O10109.91 (18)C15-C14-H14120.1O11-C11-O10109.91 (18)C15-C14-H14120.1O11-C11-O10109.91 (18)C15-C14-H16A109.5O2-Mn1-O3145.05 (8)C14-C15-H15119.6O8-Mn1-O3109.15 (8)O4-C16-H16A109.5O2-Mn1-O3145.09 (8)H16A-C16-H16A109.5O3-Mn1-O319.15 (8)O4-C16-H16A109.5O3-Mn1-O319.63 (9)H16A-C16-H16C109.5O3-Mn1-N579.31 (9	C2—C3	1.364 (4)	С38—Н38	0.9500
C3-C41.401 (5)C40-C451.383 (5)C3-H30.9500C40-C411.385 (5)C4-C51.365 (5)C41-C421.377 (5)C4-H40.9500C41-H410.9500C5-C61.412 (4)C42-C431.380 (5)C5-C61.410 (4)C43-C441.376 (5)C6-C71.410 (4)C43-C441.376 (5)C6-C81.444 (4)C43-H430.9500C8-H80.9500C44-C451.384 (5)C9-C101.480 (4)C44-H440.9500C10-C151.373 (5)C45-H450.9500C10-C111.385 (4)C46-H46B0.9800C11-C121.374 (5)C46-H46B0.9800C11-C11111.2 (3)C12-C13-H13120.0O12-C11-O11111.2 (3)C12-C13-H13120.0O12-C11-O13108.79 (19)C13-C14-C15119.8 (4)O12-C11-O10108.39 (19)C13-C14-H14120.1O11-C11-O10109.91 (18)C15-C14-H14120.1O11-C11-O10109.91 (18)C10-C15-C14120.9 (4)O2-Mn1-O3145.50 (8)C14-C15-H15119.6O2-Mn1-O3145.03 (8)C14-C16-H16A109.5O2-Mn1-O319.51 (8)O4-C16-H16A109.5O3-Mn1-O995.20 (9)O4-C16-H16A109.5O3-Mn1-O319.53 (8)C16-C1+H16C109.5O3-Mn1-N579.31 (9)H16A-C16-H16C109.5O3-Mn1-N579.31 (9)H16A-C16-H16C109.5O3-Mn1-N5	C2—C7	1.404 (4)	C39—C40	1.483 (4)
C3-H30.9500C40C411.385 (5)C4C51.365 (5)C41C421.377 (5)C4H40.9500C41H410.9500C5C61.412 (4)C42C431.380 (5)C5H50.9500C42H420.9500C6C71.410 (4)C43C441.376 (5)C6C81.444 (4)C43H430.9500C8H80.9500C44C451.384 (5)C9C101.480 (4)C44H440.9500C10C151.373 (5)C45H450.9500C10C111.385 (4)C46H46A0.9800C11C121.374 (5)C46H46B0.9800C11C121.374 (5)C14C13H13120.0O12C11O13108.7 (2)C14C13H13120.0O11C11-O13108.39 (19)C13C14C15119.8 (4)O12C11O10108.54 (18)C13C14H14120.1O11C11-O10109.91 (18)C15C14H14120.1O11C11-O10109.91 (18)C15C14H14120.9O2Mn1-O3145.50 (8)C14C15H15119.6O2Mn1-O319.15 (8)O4C16H16A109.5O2Mn1-O319.53 (9)H16AC16H16C109.5O3Mn1-N579.31 (9)H16AC16H16C109.5O3Mn1-N579.31 (9)H16AC16H16C109.5O3Mn1-N579.31 (9)H16B-C16H16C109.5O3Mn1-N579.31 (9)H16B-C16H16C109.5O3Mn1-N579.31 (9)	C3—C4	1.401 (5)	C40—C45	1.383 (5)
C4—C51.365 (5)C41—C421.377 (5)C4—H40.9500C41—H410.9500C5—C61.412 (4)C42—C431.380 (5)C5—H50.9500C42—H420.9500C6—C71.410 (4)C43—C441.376 (5)C6—C81.444 (4)C43—H430.9500C8—H80.9500C44—C451.384 (5)C9—C101.480 (4)C44—H440.9500C10—C151.373 (5)C45—H450.9500C10—C111.385 (4)C46—H46A0.9800C11—C121.374 (5)C46—H46B0.9800C11—C121.374 (5)C46—H46B0.9800C11—C11111.2 (3)C12—C13—H13120.0O12—C11—O11111.2 (3)C12—C13—H13120.0O11—C11—O13108.7 (2)C14—C13—H13120.0O11—C11—O13108.39 (19)C13—C14—C15119.8 (4)O12—C11—O10109.91 (18)C15—C14—H14120.1O11—C11—O10109.91 (18)C15—C14—H14120.1O11—C11—O10109.91 (18)C15—C14—H14120.9O2—Mn1—O3145.50 (8)C14—C15—H15119.6O2—Mn1—O319.5 (8)O4—C16—H16A109.5O2—Mn1—O319.5 (8)O4—C16—H16B109.5O3—Mn1—O319.6 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5O3—Mn1—N5 <t< td=""><td>С3—Н3</td><td>0.9500</td><td>C40—C41</td><td>1.385 (5)</td></t<>	С3—Н3	0.9500	C40—C41	1.385 (5)
C4—H40.9500C41—H410.9500C5—C61.412 (4)C42—C431.380 (5)C5—H50.9500C42—H420.9500C6—C71.410 (4)C43—C441.376 (5)C6—C81.444 (4)C43—H430.9500C8—H80.9500C44—C451.384 (5)C9—C101.480 (4)C44—H440.9500C10—C151.373 (5)C45—H450.9800C10—C111.385 (4)C46—H46A0.9800C11—C121.374 (5)C46—H46C0.9800C11—C11111.2 (3)C12—C13—H13120.0O12—C11—O11111.2 (3)C12—C13—H13120.0O12—C11—O13108.7 (2)C14—C15—H13120.0O11—C11—O13108.39 (19)C13—C14—C15119.8 (4)O12—C11—O10109.91 (18)C15—C14—H14120.1O11—C11—O10109.91 (18)C15—C14—H14120.1O13—C11—O10109.91 (8)O14—C15—H15119.6O2—Mn1—O3145.50 (8)C14—C15—H15119.6O2—Mn1—O3145.90 (8)H16A—C16—H16B109.5O2—Mn1—O319.51 (8)O4—C16—H16C109.5O3—Mn1—O319.63 (9)H16A—C16—H16C109.5O3—Mn1—O579.31 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5 <td< td=""><td>C4—C5</td><td>1.365 (5)</td><td>C41—C42</td><td>1.377 (5)</td></td<>	C4—C5	1.365 (5)	C41—C42	1.377 (5)
CSC6 $1.412 (4)$ C42C43 $1.380 (5)$ CSH5 0.9500 C42H42 0.9500 C6C7 $1.410 (4)$ C43C44 $1.376 (5)$ C6C8 $1.444 (4)$ C43H43 0.9500 C8H8 0.9500 C44C45 $1.384 (5)$ C9C10 $1.480 (4)$ C44H44 0.9500 C10C15 $1.373 (5)$ C45H45 0.9500 C10C11 $1.385 (4)$ C46H46A 0.9800 C11C12 $1.374 (5)$ C46H46B 0.9800 C11C11 $1.11.2 (3)$ C12C13H13120.0O12C11O11 $111.2 (3)$ C12C13H13120.0O12C11O13 $108.79 (19)$ C13C14C15119.8 (4)O12C11O10 $108.54 (18)$ C13C14H14120.1O11C11O10 $109.91 (18)$ C15C14H14120.1O11C11O10 $109.91 (18)$ C15C14H14120.9 (4)O2Mn1-O3 $145.50 (8)$ C10C15H15119.6O2Mn1-O3 $109.15 (8)$ O4C16H16B109.5O3Mn1-O9 $98.66 (9)$ O4C16H16B109.5O3Mn1-O9 $94.52 (9)$ O4C16H16C109.5O3Mn1-N5 $79.31 (9)$ H16AC16H16C109.5O3Mn1-N5 $71.21 (8)$ O4C17C12 $13.2 (3)$ O9Mn1-N5 $71.21 (8)$ O4C17C12 $13.2 (3)$ O3Mn1-N5 $71.21 (8)$ C18C17C12 $12.7 (3)$ O3Mn1-N1 $72.54 (8)$ C18C17C12 $12.0 5 (4)$ <	C4—H4	0.9500	C41—H41	0.9500
C5—H50.9500C42—H420.9500C6—C71.410 (4)C43—C441.376 (5)C6—C81.444 (4)C43—H430.9500C8—H80.9500C44—C451.384 (5)C9—C101.480 (4)C44—H440.9500C10—C151.373 (5)C45—H450.9500C10—C111.385 (4)C46—H46A0.9800C11—C121.374 (5)C46—H46B0.9800C11—C1111.2 (3)C12—C13—H13120.0O12—C11—O11111.2 (3)C12—C13—H13120.0O12—C11—O13108.7 (2)C14—C13—H13120.0O12—C11—O13108.39 (19)C13—C14—C15119.8 (4)O12—C11—O10109.91 (18)C13—C14—H14120.1O11—C11—O10109.91 (18)C15—C14—H14120.1O11—C11—O10109.91 (18)C15—C14—H14120.9 (4)O2—MnI—O876.87 (8)C10—C15—C14120.9 (4)O2—MnI—O3109.15 (8)O4—C16—H16A109.5O2—MnI—O998.66 (9)O4—C16—H16A109.5O3—MnI—O9143.09 (8)H16A—C16—H16B109.5O3—MnI—O995.20 (9)O4—C16—H16C109.5O3—MnI—N579.31 (9)H16B—C16—H16C109.5O3—MnI—N579.31 (9)H16B—C16—H16C109.5O3—MnI—N579.31 (9)H16B—C16—H16C109.5O3—MnI—N579.31 (9)H16B—C16—H16C109.5O3—MnI—N579.31 (9)C13—C14—C12113.2 (3)O2—MnI—N571.21 (8)C17—C22113.	C5—C6	1.412 (4)	C42—C43	1.380 (5)
C6-C71.410 (4)C43-C441.376 (5)C6-C81.444 (4)C43-H430.9500C8-H80.9500C44-C451.384 (5)C9-C101.480 (4)C44-H440.9500C10-C151.373 (5)C45-H450.9500C10-C111.385 (4)C46-H46A0.9800C11-C121.374 (5)C46-H46B0.9800C11-H110.9500C46-H46C0.9800C12-C11-O11111.2 (3)C12-C13-H13120.0O12-C11-O13108.7 (2)C14-C13-H13120.0O12-C11-O13108.39 (19)C13-C14-C15119.8 (4)O12-C11-O10109.91 (18)C15-C14-H14120.1O13-C11-O10109.91 (18)C15-C14-H14120.9O13-C11-O10109.91 (18)C15-C14-H14120.9O2-Mn1-O876.87 (8)C10-C15-H15119.6O2-Mn1-O819.5 (8)O4-C16-H16A109.5O2-Mn1-O998.66 (9)04-C16-H16B109.5O3-Mn1-O919.30 (9)H16A-C16-H16B109.5O3-Mn1-O995.20 (9)O4-C16-H16C109.5O2-Mn1-N579.31 (9)H16A-C16-H16C109.5O3-Mn1-N594.72 (9)04-C17-C12113.2 (3)O2-Mn1-N571.21 (8)C18-C17-C22113.2 (3)O2-Mn1-N571.21 (8)C18-C17-C22113.2 (3)O2-Mn1-N178.54 (8)C18-C17-C22121.7 (3)	С5—Н5	0.9500	C42—H42	0.9500
C6-C81.444 (4)C43-H430.9500C8-H80.9500C44-C451.384 (5)C9-C101.480 (4)C44-H440.9500C10-C151.373 (5)C45-H450.9800C10-C111.385 (4)C46-H46A0.9800C11-C121.374 (5)C46-H46B0.9800C12-C11-O11111.2 (3)C12-C13-H13120.0012-C11-O13108.7 (2)C14-C13-H13120.0012-C11-O13108.7 (2)C14-C13-H13120.0011-C11-O13108.39 (19)C13-C14-C15119.8 (4)012-C11-O10108.54 (18)C13-C14-H14120.1011-C11-O10109.91 (18)C15-C14-H14120.1012-C11-O10109.91 (18)C10-C15-H15119.602-Mn1-O3145.50 (8)C14-C15-H15119.602-Mn1-O319.15 (8)O4-C16-H16A109.502-Mn1-O319.51 (8)O4-C16-H16B109.503-Mn1-O995.20 (9)O4-C16-H16A109.503-Mn1-N59.31 (9)H16A-C16-H16C109.503-Mn1-N59.31 (9)H16B-C16-H16C109.503-Mn1-N59.31 (9)H16B-C16-H16C109.503-Mn1-N59.72 (9)O4-C17-C22113.2 (3)02-Mn1-N1128.89 (9)C17-C18-C19120.5 (4)03-Mn1-N1128.89 (9)C17-C18-H18119.7	C6—C7	1.410 (4)	C43—C44	1.376 (5)
C8—H80.9500C44—C451.384 (5)C9—C101.480 (4)C44—H440.9500C10—C151.373 (5)C45—H450.9500C10—C111.385 (4)C46—H46A0.9800C11—C121.374 (5)C46—H46B0.9800C11—H110.9500C46—H46C0.9800O12—C11—O11111.2 (3)C12—C13—H13120.0O12—C11—O13108.7 (2)C14—C13—H13120.0O11—C11—O13108.39 (19)C13—C14—C15119.8 (4)O12—C11—O10108.54 (18)C13—C14—H14120.1O11—C11—O10109.91 (18)C15—C14—H14120.1O13—C11—O10109.91 (18)C10—C15—C14120.9 (4)O2—Mn1—O876.87 (8)C10—C15—H15119.6O2—Mn1—O3109.15 (8)O4—C16—H16A109.5O2—Mn1—O998.66 (9)O4—C16—H16B109.5O3—Mn1—O995.20 (9)O4—C16—H16B109.5O3—Mn1—N57.9.31 (9)H16A—C16—H16C109.5O3—Mn1—N57.121 (8)O4—C17—C18125.1 (3)O9—Mn1—N57.121 (8)C18—C17—C22113.2 (3)O2—Mn1—N17.63 (8)C18—C17—C22121.7 (3)O8—Mn1—N1128.89 (9)C17—C18—H18119.7	C6—C8	1.444 (4)	С43—Н43	0.9500
C9-C10 $1.480 (4)$ C44-H44 0.9500 C10-C15 $1.373 (5)$ C45-H45 0.9500 C10-C11 $1.385 (4)$ C46-H46A 0.9800 C11-C12 $1.374 (5)$ C46-H46B 0.9800 C11-H11 0.9500 C46-H46C 0.9800 O12-C11-O11 $111.2 (3)$ C12-C13-H13 120.0 O12-C11-O13 $108.7 (2)$ C14-C13-H13 120.0 O12-C11-O13 $108.7 (2)$ C14-C13-H13 120.0 O11-C11-O13 $108.7 (2)$ C13-C14-C15 $119.8 (4)$ O12-C11-O10 $108.39 (19)$ C13-C14-H14 120.1 O11-C11-O10 $109.91 (18)$ C15-C14-H14 120.1 O11-C11-O10 $109.91 (18)$ C10-C15-C14 $120.9 (4)$ O2-Mn1-O3 $145.50 (8)$ C10-C15-H15 119.6 O2-Mn1-O3 $109.15 (8)$ O4-C16-H16A 109.5 O2-Mn1-O9 $98.66 (9)$ O4-C16-H16B 109.5 O3-Mn1-O9 $95.20 (9)$ O4-C16-H16B 109.5 O3-Mn1-N5 $79.31 (9)$ H16A-C16-H16C 109.5 O3-Mn1-N5 $71.21 (8)$ O4-C17-C18 $125.1 (3)$ O9-Mn1-N5 $71.21 (8)$ C18-C17-C22 $113.2 (3)$ O2-Mn1-N1 $72.54 (8)$ C17-C18-H18 119.7	C8—H8	0.9500	C44—C45	1.384 (5)
C10—C151.373 (5)C45—H450.9500C10—C111.385 (4)C46—H46A0.9800C11—C121.374 (5)C46—H46B0.9800C11—H110.9500C46—H46C0.9800O12—C11—O11111.2 (3)C12—C13—H13120.0O12—C11—O13108.7 (2)C14—C13—H13120.0O11—C11—O13108.39 (19)C13—C14—C15119.8 (4)O12—C11—O10108.54 (18)C13—C14—H14120.1O11—C11—O10109.91 (18)C15—C14—H14120.1O13—C11—O10110.12 (18)C10—C15—C14120.9 (4)O2—Mn1—O876.87 (8)C10—C15—H15119.6O2—Mn1—O3109.15 (8)O4—C16—H16A109.5O2—Mn1—O998.66 (9)O4—C16—H16B109.5O3—Mn1—O995.20 (9)O4—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5O3—Mn1—N571.21 (8)O4—C17—C22113.2 (3)O9—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)O3—Mn1—N172.54 (8)C17—C18—H18119.7	C9—C10	1.480 (4)	C44—H44	0.9500
C10—C111.385 (4)C46—H46A0.9800C11—C121.374 (5)C46—H46B0.9800C11—H110.9500C46—H46C0.9800O12—C11—O11111.2 (3)C12—C13—H13120.0O12—C11—O13108.7 (2)C14—C13—H13120.0O11—C11—O13108.39 (19)C13—C14—C15119.8 (4)O12—C11—O10108.54 (18)C13—C14—H14120.1O11—C11—O10109.91 (18)C15—C14—H14120.1O13—C11—O10109.91 (18)C15—C14—H14120.9 (4)O2—Mn1—O876.87 (8)C10—C15—C14120.9 (4)O2—Mn1—O3109.15 (8)O4—C16—H16A109.5O2—Mn1—O998.66 (9)O4—C16—H16B109.5O3—Mn1—O995.20 (9)O4—C16—H16C109.5O3—Mn1—N579.31 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16B—C16—H16C109.5O3—Mn1—N571.21 (8)O4—C17—C22113.2 (3)O2—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)O3—Mn1—N172.54 (8)C17—C18—H18119.7	C10—C15	1.373 (5)	C45—H45	0.9500
C11C121.374 (5)C46H46B0.9800C11H110.9500C46H46C0.9800O12C11O11111.2 (3)C12C13H13120.0O12C11O13108.7 (2)C14C13H13120.0O11C11O13108.39 (19)C13C14C15119.8 (4)O12C11O10108.54 (18)C13C14H14120.1O11C11O10109.91 (18)C15C14H14120.1O13C11O10110.12 (18)C10C15C14120.9 (4)O2Mn1-O876.87 (8)C10C15H15119.6O2Mn1-O3145.50 (8)C14C15H15119.6O2Mn1-O3109.15 (8)O4C16H16A109.5O2Mn1-O998.66 (9)O4C16H16B109.5O3Mn1-O995.20 (9)O4C16H16B109.5O3Mn1-N5119.63 (9)H16AC16H16C109.5O3Mn1-N594.72 (9)O4C17C18125.1 (3)O9Mn1-N571.21 (8)O4C17C22113.2 (3)O2Mn1-N177.63 (8)C18C17C22121.7 (3)O8Mn1-N1128.89 (9)C17C18C19120.5 (4)	C10—C11	1.385 (4)	C46—H46A	0.9800
C11—H110.9500C46—H46C0.9800012—C11—O11111.2 (3)C12—C13—H13120.0012—C11—O13108.7 (2)C14—C13—H13120.0011—C11—O13108.39 (19)C13—C14—C15119.8 (4)012—C11—O10108.54 (18)C13—C14—H14120.1011—C11—O10109.91 (18)C15—C14—H14120.1013—C11—O10110.12 (18)C10—C15—C14120.9 (4)02—Mn1—O876.87 (8)C10—C15—H15119.602—Mn1—O3145.50 (8)C14—C15—H15119.603—Mn1—O998.66 (9)O4—C16—H16A109.503—Mn1—O9143.09 (8)H16A—C16—H16B109.503—Mn1—N5119.63 (9)H16A—C16—H16C109.503—Mn1—N594.72 (9)O4—C17—C18125.1 (3)09—Mn1—N571.21 (8)O4—C17—C22113.2 (3)02—Mn1—N177.63 (8)C18—C17—C22121.7 (3)03—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)03—Mn1—N172.54 (8)C17—C18—H18119.7	C11—C12	1.374 (5)	С46—Н46В	0.9800
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11—H11	0.9500	С46—Н46С	0.9800
012—C11—013108.7 (2)C14—C13—H13120.0011—C11—013108.39 (19)C13—C14—C15119.8 (4)012—C11—010108.54 (18)C13—C14—H14120.1011—C11—010109.91 (18)C15—C14—H14120.9 (4)02—Mn1—0876.87 (8)C10—C15—C14120.9 (4)02—Mn1—03145.50 (8)C14—C15—H15119.608—Mn1—03109.15 (8)04—C16—H16A109.502—Mn1—0998.66 (9)04—C16—H16B109.503—Mn1—09143.09 (8)H16A—C16—H16C109.503—Mn1—N5119.63 (9)H16B—C16—H16C109.503—Mn1—N579.31 (9)H16B—C16—H16C109.503—Mn1—N571.21 (8)04—C17—C18125.1 (3)09—Mn1—N177.63 (8)C18—C17—C22113.2 (3)03—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)03—Mn1—N172.54 (8)C17—C18—H18119.7	O12—C11—O11	111.2 (3)	C12—C13—H13	120.0
011Cl1013108.39 (19)C13Cl4Cl5119.8 (4)012Cl1010108.54 (18)C13Cl4H14120.1011Cl1010109.91 (18)C15Cl4H14120.9 (4)02Mn1-0876.87 (8)C10Cl5Cl4120.9 (4)02Mn1-03145.50 (8)C14Cl5H15119.602Mn1-03109.15 (8)04Cl6H16A109.502Mn1-0998.66 (9)04Cl6H16B109.503Mn1-0995.20 (9)04Cl6H16B109.503Mn1-N5119.63 (9)H16ACl6H16C109.503Mn1-N594.72 (9)04Cl7Cl8125.1 (3)09Mn1-N571.21 (8)04Cl7Cl22113.2 (3)02Mn1-N177.63 (8)C18Cl7C22121.7 (3)03Mn1-N1128.89 (9)Cl7Cl8H18119.7	O12-C11-O13	108.7 (2)	C14—C13—H13	120.0
012C11010108.54 (18)C13C14H14120.1011C11010109.91 (18)C15C14H14120.9 (4)02Mn10876.87 (8)C10C15C14120.9 (4)02Mn103145.50 (8)C14C15H15119.608Mn103109.15 (8)04C16H16A109.502Mn10998.66 (9)04C16H16B109.503Mn1-09143.09 (8)H16AC16H16B109.503Mn1-0995.20 (9)04C16H16C109.502Mn1-N5119.63 (9)H16AC16H16C109.503Mn1-N594.72 (9)04C17C18125.1 (3)09Mn1-N571.21 (8)04C17C22113.2 (3)02Mn1-N1128.89 (9)C17C18C19120.5 (4)03Mn1-N172.54 (8)C17C18H18119.7	O11—Cl1—O13	108.39 (19)	C13—C14—C15	119.8 (4)
O11—C11—O10109.91 (18)C15—C14—H14120.1O13—C11—O10110.12 (18)C10—C15—C14120.9 (4)O2—Mn1—O876.87 (8)C10—C15—H15119.6O2—Mn1—O3145.50 (8)C14—C15—H15119.6O8—Mn1—O3109.15 (8)O4—C16—H16A109.5O2—Mn1—O998.66 (9)O4—C16—H16B109.5O3—Mn1—O995.20 (9)O4—C16—H16B109.5O2—Mn1—N5119.63 (9)H16A—C16—H16C109.5O3—Mn1—N594.72 (9)O4—C17—C18125.1 (3)O9—Mn1—N571.21 (8)O4—C17—C22113.2 (3)O2—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)O3—Mn1—N172.54 (8)C17—C18—H18119.7	O12-Cl1-O10	108.54 (18)	C13—C14—H14	120.1
O13—C11—O10110.12 (18)C10—C15—C14120.9 (4)O2—Mn1—O876.87 (8)C10—C15—H15119.6O2—Mn1—O3145.50 (8)C14—C15—H15119.6O8—Mn1—O3109.15 (8)O4—C16—H16A109.5O2—Mn1—O998.66 (9)O4—C16—H16B109.5O8—Mn1—O9143.09 (8)H16A—C16—H16B109.5O3—Mn1—O995.20 (9)O4—C16—H16C109.5O2—Mn1—N5119.63 (9)H16A—C16—H16C109.5O3—Mn1—N579.31 (9)H16B—C16—H16C109.5O3—Mn1—N594.72 (9)O4—C17—C18125.1 (3)O9—Mn1—N571.21 (8)O4—C17—C22113.2 (3)O2—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)O3—Mn1—N172.54 (8)C17—C18—H18119.7	O11—Cl1—O10	109.91 (18)	C15-C14-H14	120.1
O2-Mn1-O876.87 (8)C10-C15-H15119.6O2-Mn1-O3145.50 (8)C14-C15-H15119.6O8-Mn1-O3109.15 (8)O4-C16-H16A109.5O2-Mn1-O998.66 (9)O4-C16-H16B109.5O8-Mn1-O9143.09 (8)H16A-C16-H16B109.5O3-Mn1-O995.20 (9)O4-C16-H16C109.5O2-Mn1-N5119.63 (9)H16A-C16-H16C109.5O3-Mn1-N579.31 (9)H16B-C16-H16C109.5O3-Mn1-N594.72 (9)O4-C17-C18125.1 (3)O9-Mn1-N571.21 (8)O4-C17-C22113.2 (3)O2-Mn1-N177.63 (8)C18-C17-C22121.7 (3)O8-Mn1-N1128.89 (9)C17-C18-C19120.5 (4)O3-Mn1-N172.54 (8)C17-C18-H18119.7	O13-Cl1-O10	110.12 (18)	C10-C15-C14	120.9 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—Mn1—O8	76.87 (8)	C10-C15-H15	119.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—Mn1—O3	145.50 (8)	C14—C15—H15	119.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O8—Mn1—O3	109.15 (8)	O4—C16—H16A	109.5
O8—Mn1—O9143.09 (8)H16A—C16—H16B109.5O3—Mn1—O995.20 (9)O4—C16—H16C109.5O2—Mn1—N5119.63 (9)H16A—C16—H16C109.5O8—Mn1—N579.31 (9)H16B—C16—H16C109.5O3—Mn1—N594.72 (9)O4—C17—C18125.1 (3)O9—Mn1—N571.21 (8)O4—C17—C22113.2 (3)O2—Mn1—N177.63 (8)C18—C17—C22121.7 (3)O8—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)O3—Mn1—N172.54 (8)C17—C18—H18119.7	O2—Mn1—O9	98.66 (9)	O4—C16—H16B	109.5
O3—Mn1—O995.20 (9)O4—C16—H16C109.5O2—Mn1—N5119.63 (9)H16A—C16—H16C109.5O8—Mn1—N579.31 (9)H16B—C16—H16C109.5O3—Mn1—N594.72 (9)O4—C17—C18125.1 (3)O9—Mn1—N571.21 (8)O4—C17—C22113.2 (3)O2—Mn1—N177.63 (8)C18—C17—C22121.7 (3)O8—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)O3—Mn1—N172.54 (8)C17—C18—H18119.7	O8—Mn1—O9	143.09 (8)	H16A—C16—H16B	109.5
O2Mn1N5119.63 (9)H16AC16H16C109.5O8Mn1N579.31 (9)H16BC16H16C109.5O3Mn1N594.72 (9)O4C17C18125.1 (3)O9Mn1N571.21 (8)O4C17C22113.2 (3)O2Mn1N177.63 (8)C18C17C22121.7 (3)O8Mn1N1128.89 (9)C17C18C19120.5 (4)O3Mn1N172.54 (8)C17C18H18119.7	O3—Mn1—O9	95.20 (9)	O4—C16—H16C	109.5
O8—Mn1—N579.31 (9)H16B—C16—H16C109.5O3—Mn1—N594.72 (9)O4—C17—C18125.1 (3)O9—Mn1—N571.21 (8)O4—C17—C22113.2 (3)O2—Mn1—N177.63 (8)C18—C17—C22121.7 (3)O8—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)O3—Mn1—N172.54 (8)C17—C18—H18119.7	O2—Mn1—N5	119.63 (9)	H16A—C16—H16C	109.5
O3-Mn1-N594.72 (9)O4-C17-C18125.1 (3)O9-Mn1-N571.21 (8)O4-C17-C22113.2 (3)O2-Mn1-N177.63 (8)C18-C17-C22121.7 (3)O8-Mn1-N1128.89 (9)C17-C18-C19120.5 (4)O3-Mn1-N172.54 (8)C17-C18-H18119.7	O8—Mn1—N5	79.31 (9)	H16B—C16—H16C	109.5
O9-Mn1-N571.21 (8)O4-C17-C22113.2 (3)O2-Mn1-N177.63 (8)C18-C17-C22121.7 (3)O8-Mn1-N1128.89 (9)C17-C18-C19120.5 (4)O3-Mn1-N172.54 (8)C17-C18-H18119.7	O3—Mn1—N5	94.72 (9)	O4—C17—C18	125.1 (3)
O2-Mn1-N177.63 (8)C18-C17-C22121.7 (3)O8-Mn1-N1128.89 (9)C17-C18-C19120.5 (4)O3-Mn1-N172.54 (8)C17-C18-H18119.7	O9—Mn1—N5	71.21 (8)	O4—C17—C22	113.2 (3)
O8—Mn1—N1128.89 (9)C17—C18—C19120.5 (4)O3—Mn1—N172.54 (8)C17—C18—H18119.7	O2—Mn1—N1	77.63 (8)	C18—C17—C22	121.7 (3)
O3—Mn1—N1 72.54 (8) C17—C18—H18 119.7	O8—Mn1—N1	128.89 (9)	C17—C18—C19	120.5 (4)
	O3—Mn1—N1	72.54 (8)	C17—C18—H18	119.7

O9—Mn1—N1	84.16 (8)	C19—C18—H18	119.7
N5—Mn1—N1	151.29 (9)	C20—C19—C18	119.1 (3)
O5—Mn2—O2	109.55 (9)	С20—С19—Н19	120.4
O5—Mn2—O6	150.92 (8)	С18—С19—Н19	120.4
O2—Mn2—O6	96.68 (8)	C19—C20—C21	122.2 (3)
O5—Mn2—N3	82.02 (9)	С19—С20—Н20	118.9
O2—Mn2—N3	168.30 (9)	С21—С20—Н20	118.9
O6—Mn2—N3	72.45 (9)	C20—C21—C22	119.4 (3)
O5—Mn2—O8	107.68 (8)	C20—C21—C23	117.0 (3)
O2—Mn2—O8	74.83 (8)	C22—C21—C23	123.5 (3)
O6—Mn2—O8	90.80 (8)	O5—C22—C17	118.9 (3)
N3—Mn2—O8	100.50 (9)	O5—C22—C21	124.1 (3)
O5—Mn2—O1	92.92 (9)	C17—C22—C21	117.0 (3)
O2—Mn2—O1	68.95 (8)	N3—C23—C21	124.6 (3)
O6—Mn2—O1	84.77 (8)	N3—C23—H23	117.7
N3—Mn2—O1	113.22 (9)	С21—С23—Н23	117.7
O8—Mn2—O1	142.67 (7)	O6—C24—N4	120.1 (3)
C8—N1—N2	117.0 (2)	O6—C24—C25	121.8 (3)
C8—N1—Mn1	131.2 (2)	N4—C24—C25	118.1 (3)
N2—N1—Mn1	111.15 (17)	C26—C25—C30	118.8 (3)
C9—N2—N1	116.7 (2)	C26—C25—C24	123.2 (3)
C9—N2—H2A	121.6	C30—C25—C24	117.9 (3)
N1—N2—H2A	121.6	C27—C26—C25	119.8 (3)
C23—N3—N4	117.4 (3)	С27—С26—Н26	120.1
C23—N3—Mn2	130.8 (2)	С25—С26—Н26	120.1
N4—N3—Mn2	111.61 (18)	C28—C27—C26	120.5 (4)
C24—N4—N3	116.6 (2)	С28—С27—Н27	119.7
C24—N4—H4A	121.7	С26—С27—Н27	119.7
N3—N4—H4A	121.7	C29—C28—C27	120.7 (4)
C38—N5—N6	116.8 (3)	C29—C28—H28	119.7
C38—N5—Mn1	130.1 (2)	C27—C28—H28	119.7
N6—N5—Mn1	113.08 (18)	C28—C29—C30	119.0 (4)
C39—N6—N5	116.4 (3)	С28—С29—Н29	120.5
C39—N6—H6A	121.8	С30—С29—Н29	120.5
N5—N6—H6A	121.8	C29—C30—C25	121.2 (4)
C2—O1—C1	118.0 (3)	С29—С30—Н30	119.4
C2—O1—Mn2	111.43 (18)	С25—С30—Н30	119.4
C1—O1—Mn2	130.5 (2)	O7—C31—H31A	109.5
C7—O2—Mn2	122.82 (18)	O7—C31—H31B	109.5
C7—O2—Mn1	133.25 (18)	H31A—C31—H31B	109.5
Mn2—O2—Mn1	103.50 (9)	O7—C31—H31C	109.5
C9—O3—Mn1	118.2 (2)	H31A—C31—H31C	109.5
C17—O4—C16	118.2 (3)	H31B—C31—H31C	109.5
C22—O5—Mn2	133.1 (2)	O7—C32—C33	125.0 (3)
C24—O6—Mn2	114.7 (2)	O7—C32—C37	113.9 (3)
C32—O7—C31	117.1 (3)	C33—C32—C37	121.1 (3)
C37—O8—Mn1	131.7 (2)	C32—C33—C34	120.5 (3)
C37—O8—Mn2	116.67 (18)	С32—С33—Н33	119.8
Mn1—O8—Mn2	98.92 (8)	С34—С33—Н33	119.8

C39—O9—Mn1	118.4 (2)	C35—C34—C33	120.3 (3)
C46—O14—H14A	109.5	С35—С34—Н34	119.8
O1—C1—H1A	109.5	С33—С34—Н34	119.8
O1—C1—H1B	109.5	C34—C35—C36	120.9 (3)
H1A—C1—H1B	109.5	С34—С35—Н35	119.5
01—C1—H1C	109.5	С36—С35—Н35	119.5
H1A—C1—H1C	109.5	C35—C36—C37	119.6 (3)
H1B—C1—H1C	109.5	C35—C36—C38	117.0 (3)
C3—C2—O1	125.1 (3)	C37—C36—C38	123.4 (3)
C3—C2—C7	122.3 (3)	O8—C37—C36	123.1 (3)
O1—C2—C7	112.5 (3)	O8—C37—C32	119.3 (3)
C2—C3—C4	118.8 (3)	C36—C37—C32	117.5 (3)
С2—С3—Н3	120.6	N5—C38—C36	124.2 (3)
С4—С3—Н3	120.6	N5—C38—H38	117.9
C5—C4—C3	120.6 (3)	С36—С38—Н38	117.9
С5—С4—Н4	119.7	O9—C39—N6	120.1 (3)
С3—С4—Н4	119.7	O9—C39—C40	120.6 (3)
C4—C5—C6	121.3 (3)	N6—C39—C40	119.3 (3)
С4—С5—Н5	119.4	C45—C40—C41	119.6 (3)
С6—С5—Н5	119.4	C45—C40—C39	117.0 (3)
C7—C6—C5	118.3 (3)	C41—C40—C39	123.4 (3)
C7—C6—C8	123.4 (3)	C42—C41—C40	119.7 (4)
C5—C6—C8	118.3 (3)	C42—C41—H41	120.1
O2—C7—C2	118.6 (3)	C40—C41—H41	120.1
O2—C7—C6	122.7 (3)	C41—C42—C43	120.6 (4)
C2—C7—C6	118.7 (3)	C41—C42—H42	119.7
N1—C8—C6	123.4 (3)	C43—C42—H42	119.7
N1—C8—H8	118.3	C44—C43—C42	120.1 (3)
С6—С8—Н8	118.3	C44—C43—H43	120.0
O3—C9—N2	120.9 (3)	C42—C43—H43	120.0
O3—C9—C10	120.8 (3)	C43—C44—C45	119.5 (3)
N2—C9—C10	118.3 (3)	C43—C44—H44	120.3
C15-C10-C11	118.0 (3)	C45—C44—H44	120.3
C15—C10—C9	117.9 (3)	C40—C45—C44	120.5 (3)
C11—C10—C9	124.0 (3)	C40—C45—H45	119.7
C12-C11-C10	120.7 (3)	C44—C45—H45	119.7
C12-C11-H11	119.6	O14—C46—H46A	109.5
C10-C11-H11	119.6	O14—C46—H46B	109.5
C13—C12—C11	120.4 (4)	H46A—C46—H46B	109.5
C13—C12—H12	119.8	O14—C46—H46C	109.5
C11—C12—H12	119.8	H46A—C46—H46C	109.5
C12—C13—C14	120.1 (4)	H46B—C46—H46C	109.5

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A
N2—H2A···O5 ⁱ	0.88	2.04	2.907 (3)	168
N4—H4A···O13 ⁱⁱ	0.88	2.08	2.910 (4)	156
N6—H6A…O14	0.88	1.98	2.810 (4)	156

O14—H14A···O10ⁱⁱⁱ 0.84 2.05 2.865 (4) 165 Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x+1, -y+2, -z+1; (iii) x-1, y, z.

Fig. 1







