

# Chlorido(chlorodifluoroacetato- $\kappa$ O)-bis(1,10-phenanthroline- $\kappa^2$ N,N')-manganese(II)

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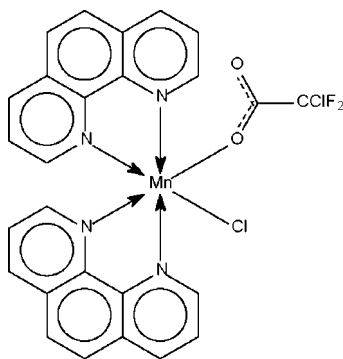
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.057;  $wR$  factor = 0.165; data-to-parameter ratio = 16.9.

The chloride and chlorodifluoroacetate anions occupy *cis* positions in the octahedral coordination geometry of the title compound,  $[\text{Mn}(\text{C}_2\text{ClF}_2\text{O}_2)\text{Cl}(\text{C}_{12}\text{H}_8\text{N}_2)_2]$ . The two *N*-heterocycles both chelate the metal atom.

## Related literature

For isostructural chlorido(1,10-phenanthroline)(trichloroacetato)manganese(II), see: Chen *et al.* (2006).



## Experimental

### Crystal data

 $[\text{Mn}(\text{C}_2\text{ClF}_2\text{O}_2)\text{Cl}(\text{C}_{12}\text{H}_8\text{N}_2)_2]$ 
 $M_r = 580.27$ Monoclinic,  $P2_1/c$  $a = 16.8822$  (4) Å $b = 10.3781$  (3) Å $c = 14.8364$  (5) Å $\beta = 108.813$  (2)° $V = 2460.5$  (1) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.80$  mm<sup>-1</sup> $T = 100$  (2) K

0.20 × 0.15 × 0.10 mm

### Data collection

Bruker SMART APEXII

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.856$ ,  $T_{\max} = 0.924$ 

30077 measured reflections

5628 independent reflections

3863 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.104$ 

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.057$  $wR(F^2) = 0.165$  $S = 1.04$ 

5628 reflections

334 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 1.00$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.63$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Mn1—O1	2.143 (2)	Mn1—N3	2.305 (3)
Mn1—N1	2.283 (3)	Mn1—N4	2.295 (3)
Mn1—N2	2.277 (3)	Mn1—Cl1	2.443 (1)
O1—Mn1—N1	110.1 (1)	N1—Mn1—Cl1	90.4 (1)
O1—Mn1—N2	88.1 (1)	N2—Mn1—N3	93.0 (1)
O1—Mn1—N3	82.9 (1)	N2—Mn1—N4	85.2 (1)
O1—Mn1—N4	153.8 (1)	N2—Mn1—Cl1	162.7 (1)
O1—Mn1—Cl1	101.1 (1)	N3—Mn1—N4	72.2 (1)
N1—Mn1—N2	72.6 (1)	N3—Mn1—Cl1	102.6 (1)
N1—Mn1—N3	159.7 (1)	N4—Mn1—Cl1	92.4 (1)
N1—Mn1—N4	92.1 (1)		

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2008).

The authors thank the University of Malaya for funding this study (grant No. SF022155/2007A) and also for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2236).

## References

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**supplementary materials**

*Acta Cryst.* (2008). E64, m709 [ doi:10.1107/S1600536808010829 ]

**Chlorido(chlorodifluoroacetato- $\kappa O$ )bis(1,10-phenanthroline- $\kappa^2 N, N'$ )manganese(II)**

**K. M. Lo and S. W. Ng**

**Comment**

Manganese dichloride typically reacts with carboxylate anions in the presence of a neutral  $\alpha, \alpha$ -diamine ligand (such as 1,10-phenanthroline) to furnish the expected manganese dicarboxylate as the 1:2 adduct of the  $N$ -heterocycle. In the case of the reaction with the trichloroacetate anion, only one chloride is displaced. Chlorido-bis(1,10-phenanthroline)(trichloroacetato)manganese exists as a monomeric compound; the crystal structure displays  $\pi$ - $\pi$  interactions that appear to stabilize the structure (Chen *et al.*, 2006). Replacing the trichloroacetate anion by the chlorodifluoroacetate anion furnishes an isostructural compound (Scheme I, Fig. 1).

**Experimental**

Manganese dichloride dihydrate (0.5 g, 3 mmol) was dissolved in ethanol and chlorodifluoroacetic acid (0.3 ml, 3 mol) was added. The mixture was heated briefly, after which 1,10-phenanthroline (1.6 g, 6 mmol) was added. The solution when allowed to cool yielded yellow crystals.

**Refinement**

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with  $U(H)$  set to  $1.2U_{eq}(C)$ .

**Figures**

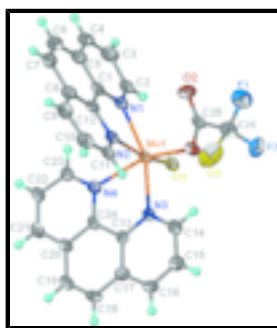


Fig. 1. 70% Probability thermal ellipsoid plot (Barbour, 2001) of  $Mn(C_{12}H_8N_2)_2(C_2ClF_2O_2)Cl$ . Hydrogen atoms are drawn as spheres of arbitrary radii.

**Chlorido(chlorodifluoroacetato- $\kappa O$ )bis(1,10-phenanthroline-  $\kappa^2 N, N'$ )manganese(II)**

*Crystal data*

$[Mn(C_2ClF_2O_2)Cl(C_{12}H_8N_2)_2]$

$M_r = 580.27$

$F_{000} = 1172$

$D_x = 1.566 \text{ Mg m}^{-3}$

# supplementary materials

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Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 16.8822$  (4) Å

$b = 10.3781$  (3) Å

$c = 14.8364$  (5) Å

$\beta = 108.813$  (2)°

$V = 2460.5$  (1) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 2908 reflections

$\theta = 2.3$ – $21.4$ °

$\mu = 0.80$  mm<sup>-1</sup>

$T = 100$  (2) K

Irregular block, yellow

$0.20 \times 0.15 \times 0.10$  mm

## Data collection

Bruker SMART APEX  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 100$ (2) K

$\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.856$ ,  $T_{\max} = 0.924$

30077 measured reflections

5628 independent reflections

3863 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.104$

$\theta_{\max} = 27.5$ °

$\theta_{\min} = 1.3$ °

$h = -21 \rightarrow 21$

$k = -13 \rightarrow 13$

$l = -19 \rightarrow 14$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.165$

$S = 1.04$

5628 reflections

334 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0868P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.00$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.62$  e Å<sup>-3</sup>

Extinction correction: none

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.28449 (3)	0.63507 (5)	0.17308 (4)	0.02130 (16)
Cl1	0.33600 (5)	0.60920 (8)	0.03799 (6)	0.0247 (2)
Cl2	0.21097 (8)	1.04489 (11)	0.29372 (9)	0.0536 (3)
F1	0.09738 (14)	1.0724 (2)	0.1347 (2)	0.0545 (8)
F2	0.22337 (14)	1.0904 (2)	0.13132 (18)	0.0402 (6)
O1	0.24710 (14)	0.8334 (2)	0.15829 (18)	0.0264 (6)
O2	0.10701 (14)	0.8221 (2)	0.1178 (2)	0.0330 (6)
N1	0.17254 (16)	0.5061 (3)	0.1004 (2)	0.0240 (6)

N2	0.21023 (16)	0.6109 (3)	0.2757 (2)	0.0230 (6)
N3	0.39971 (15)	0.7160 (3)	0.2897 (2)	0.0219 (6)
N4	0.36197 (16)	0.4637 (3)	0.2525 (2)	0.0215 (6)
C1	0.1249 (2)	0.4714 (3)	0.1547 (3)	0.0239 (7)
C2	0.1524 (2)	0.4572 (3)	0.0131 (3)	0.0275 (8)
H2	0.1857	0.4800	-0.0254	0.033*
C3	0.0848 (2)	0.3739 (3)	-0.0250 (3)	0.0338 (9)
H3	0.0720	0.3432	-0.0885	0.041*
C4	0.0376 (2)	0.3369 (3)	0.0295 (3)	0.0312 (9)
H4	-0.0080	0.2793	0.0049	0.037*
C5	0.0572 (2)	0.3857 (3)	0.1237 (3)	0.0279 (8)
C6	0.0103 (2)	0.3542 (3)	0.1854 (3)	0.0328 (9)
H6	-0.0356	0.2963	0.1638	0.039*
C7	0.0297 (2)	0.4050 (4)	0.2738 (3)	0.0313 (9)
H7	-0.0018	0.3813	0.3140	0.038*
C8	0.0975 (2)	0.4944 (3)	0.3072 (3)	0.0266 (8)
C9	0.1187 (2)	0.5535 (3)	0.3974 (3)	0.0294 (8)
H9	0.0885	0.5332	0.4397	0.035*
C10	0.1829 (2)	0.6399 (3)	0.4236 (3)	0.0316 (8)
H10	0.1973	0.6819	0.4836	0.038*
C11	0.2276 (2)	0.6658 (3)	0.3604 (3)	0.0248 (7)
H11	0.2724	0.7257	0.3795	0.030*
C12	0.14495 (19)	0.5264 (3)	0.2484 (3)	0.0228 (7)
C13	0.45711 (19)	0.6274 (3)	0.3381 (2)	0.0217 (7)
C14	0.4167 (2)	0.8390 (3)	0.3096 (3)	0.0274 (8)
H14	0.3766	0.9014	0.2767	0.033*
C15	0.4910 (2)	0.8821 (3)	0.3767 (3)	0.0299 (8)
H15	0.5006	0.9716	0.3891	0.036*
C16	0.5496 (2)	0.7935 (3)	0.4243 (3)	0.0282 (8)
H16	0.6007	0.8210	0.4696	0.034*
C17	0.5338 (2)	0.6622 (3)	0.4060 (3)	0.0251 (8)
C18	0.5921 (2)	0.5629 (3)	0.4517 (3)	0.0291 (8)
H18	0.6446	0.5861	0.4962	0.035*
C19	0.5738 (2)	0.4374 (3)	0.4329 (3)	0.0280 (8)
H19	0.6135	0.3737	0.4643	0.034*
C20	0.4951 (2)	0.3985 (3)	0.3662 (3)	0.0241 (7)
C21	0.4724 (2)	0.2692 (3)	0.3466 (3)	0.0271 (8)
H21	0.5097	0.2025	0.3778	0.033*
C22	0.3961 (2)	0.2393 (3)	0.2822 (3)	0.0284 (8)
H22	0.3795	0.1520	0.2689	0.034*
C23	0.3430 (2)	0.3395 (3)	0.2362 (3)	0.0249 (8)
H23	0.2906	0.3178	0.1909	0.030*
C24	0.43732 (19)	0.4937 (3)	0.3181 (2)	0.0211 (7)
C25	0.1748 (2)	0.8752 (3)	0.1456 (2)	0.0234 (7)
C26	0.1740 (2)	1.0211 (3)	0.1694 (3)	0.0330 (9)

## supplementary materials

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### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mn1	0.0192 (3)	0.0265 (3)	0.0161 (3)	-0.00035 (19)	0.0028 (2)	-0.0001 (2)
C11	0.0231 (4)	0.0310 (4)	0.0189 (5)	0.0005 (3)	0.0053 (3)	0.0006 (3)
C12	0.0682 (7)	0.0614 (7)	0.0398 (7)	-0.0225 (6)	0.0291 (6)	-0.0250 (5)
F1	0.0351 (12)	0.0376 (13)	0.086 (2)	0.0129 (10)	0.0131 (13)	0.0026 (13)
F2	0.0446 (13)	0.0359 (12)	0.0427 (16)	-0.0083 (10)	0.0178 (11)	0.0021 (11)
O1	0.0224 (12)	0.0323 (13)	0.0221 (14)	0.0033 (9)	0.0038 (10)	0.0028 (10)
O2	0.0236 (12)	0.0375 (14)	0.0354 (17)	-0.0043 (10)	0.0061 (12)	-0.0090 (12)
N1	0.0213 (13)	0.0294 (15)	0.0185 (16)	0.0014 (11)	0.0024 (12)	-0.0009 (12)
N2	0.0199 (13)	0.0282 (15)	0.0185 (16)	0.0015 (11)	0.0028 (12)	0.0013 (12)
N3	0.0200 (13)	0.0265 (15)	0.0174 (16)	-0.0022 (11)	0.0036 (12)	0.0019 (11)
N4	0.0207 (13)	0.0280 (15)	0.0158 (16)	-0.0024 (11)	0.0057 (12)	-0.0013 (11)
C1	0.0208 (15)	0.0279 (17)	0.0204 (19)	0.0042 (13)	0.0032 (14)	0.0028 (14)
C2	0.0279 (17)	0.0340 (19)	0.017 (2)	-0.0003 (14)	0.0022 (15)	-0.0027 (15)
C3	0.034 (2)	0.037 (2)	0.024 (2)	-0.0029 (16)	0.0000 (17)	-0.0069 (16)
C4	0.0240 (17)	0.0299 (19)	0.032 (2)	-0.0014 (14)	-0.0015 (16)	-0.0027 (16)
C5	0.0242 (17)	0.0295 (18)	0.025 (2)	0.0015 (14)	0.0017 (15)	-0.0007 (15)
C6	0.0222 (17)	0.035 (2)	0.037 (2)	-0.0039 (14)	0.0042 (17)	0.0015 (17)
C7	0.0267 (18)	0.037 (2)	0.033 (2)	0.0002 (15)	0.0130 (17)	0.0044 (17)
C8	0.0221 (16)	0.0308 (18)	0.025 (2)	0.0011 (14)	0.0044 (15)	0.0028 (15)
C9	0.0291 (18)	0.040 (2)	0.020 (2)	0.0007 (15)	0.0101 (16)	0.0041 (16)
C10	0.0336 (19)	0.040 (2)	0.020 (2)	0.0023 (16)	0.0070 (16)	-0.0016 (16)
C11	0.0225 (16)	0.0343 (18)	0.0140 (18)	-0.0009 (13)	0.0009 (14)	-0.0014 (14)
C12	0.0177 (15)	0.0279 (17)	0.0197 (19)	0.0032 (13)	0.0018 (14)	0.0015 (14)
C13	0.0211 (15)	0.0271 (17)	0.0172 (18)	-0.0006 (13)	0.0067 (14)	0.0018 (14)
C14	0.0259 (17)	0.0265 (18)	0.028 (2)	-0.0006 (13)	0.0063 (16)	0.0005 (15)
C15	0.0263 (17)	0.0292 (18)	0.030 (2)	-0.0073 (14)	0.0042 (16)	-0.0041 (16)
C16	0.0240 (16)	0.0343 (19)	0.024 (2)	-0.0074 (14)	0.0048 (15)	-0.0008 (15)
C17	0.0229 (16)	0.0341 (19)	0.0187 (19)	-0.0043 (14)	0.0071 (15)	0.0009 (15)
C18	0.0202 (16)	0.037 (2)	0.025 (2)	-0.0021 (14)	0.0003 (15)	-0.0001 (16)
C19	0.0235 (16)	0.0338 (19)	0.022 (2)	0.0043 (14)	0.0014 (15)	0.0031 (15)
C20	0.0209 (16)	0.0340 (18)	0.0159 (18)	0.0020 (14)	0.0042 (14)	0.0017 (14)
C21	0.0263 (17)	0.0274 (18)	0.026 (2)	0.0048 (14)	0.0061 (15)	0.0028 (15)
C22	0.0268 (17)	0.0271 (18)	0.028 (2)	0.0018 (14)	0.0047 (15)	0.0000 (15)
C23	0.0213 (16)	0.0295 (18)	0.023 (2)	-0.0012 (13)	0.0055 (15)	0.0006 (14)
C24	0.0206 (15)	0.0303 (17)	0.0134 (17)	0.0002 (13)	0.0070 (13)	0.0025 (13)
C25	0.0224 (16)	0.0364 (19)	0.0107 (17)	0.0001 (14)	0.0045 (14)	0.0008 (14)
C26	0.0266 (17)	0.037 (2)	0.035 (2)	0.0007 (15)	0.0089 (17)	-0.0015 (17)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Mn1—O1	2.143 (2)	C7—C8	1.432 (5)
Mn1—N1	2.283 (3)	C7—H7	0.9500
Mn1—N2	2.277 (3)	C8—C12	1.401 (5)
Mn1—N3	2.305 (3)	C8—C9	1.410 (5)
Mn1—N4	2.295 (3)	C9—C10	1.363 (5)

Mn1—C11	2.443 (1)	C9—H9	0.9500
C12—C26	1.764 (4)	C10—C11	1.405 (5)
F1—C26	1.339 (4)	C10—H10	0.9500
F2—C26	1.355 (4)	C11—H11	0.9500
O1—C25	1.250 (4)	C13—C17	1.407 (5)
O2—C25	1.217 (4)	C13—C24	1.436 (4)
N1—C2	1.330 (5)	C14—C15	1.400 (5)
N1—C1	1.358 (5)	C14—H14	0.9500
N2—C11	1.324 (5)	C15—C16	1.368 (5)
N2—C12	1.363 (4)	C15—H15	0.9500
N3—C14	1.321 (4)	C16—C17	1.398 (5)
N3—C13	1.361 (4)	C16—H16	0.9500
N4—C23	1.331 (4)	C17—C18	1.436 (5)
N4—C24	1.365 (4)	C18—C19	1.346 (5)
C1—C5	1.403 (5)	C18—H18	0.9500
C1—C12	1.440 (5)	C19—C20	1.435 (5)
C2—C3	1.398 (5)	C19—H19	0.9500
C2—H2	0.9500	C20—C21	1.399 (5)
C3—C4	1.362 (6)	C20—C24	1.410 (4)
C3—H3	0.9500	C21—C22	1.369 (5)
C4—C5	1.422 (5)	C21—H21	0.9500
C4—H4	0.9500	C22—C23	1.398 (5)
C5—C6	1.428 (6)	C22—H22	0.9500
C6—C7	1.353 (6)	C23—H23	0.9500
C6—H6	0.9500	C25—C26	1.556 (5)
O1—Mn1—N1	110.1 (1)	C9—C10—C11	119.0 (4)
O1—Mn1—N2	88.1 (1)	C9—C10—H10	120.5
O1—Mn1—N3	82.9 (1)	C11—C10—H10	120.5
O1—Mn1—N4	153.8 (1)	N2—C11—C10	123.3 (3)
O1—Mn1—C11	101.1 (1)	N2—C11—H11	118.4
N1—Mn1—N2	72.6 (1)	C10—C11—H11	118.3
N1—Mn1—N3	159.7 (1)	N2—C12—C8	122.5 (3)
N1—Mn1—N4	92.1 (1)	N2—C12—C1	117.2 (3)
N1—Mn1—C11	90.4 (1)	C8—C12—C1	120.2 (3)
N2—Mn1—N3	93.0 (1)	N3—C13—C17	122.6 (3)
N2—Mn1—N4	85.2 (1)	N3—C13—C24	117.8 (3)
N2—Mn1—C11	162.7 (1)	C17—C13—C24	119.7 (3)
N3—Mn1—N4	72.2 (1)	N3—C14—C15	123.2 (3)
N3—Mn1—C11	102.6 (1)	N3—C14—H14	118.4
N4—Mn1—C11	92.4 (1)	C15—C14—H14	118.4
C25—O1—Mn1	126.1 (2)	C16—C15—C14	119.0 (3)
C2—N1—C1	117.6 (3)	C16—C15—H15	120.5
C2—N1—Mn1	126.6 (2)	C14—C15—H15	120.5
C1—N1—Mn1	115.7 (2)	C15—C16—C17	119.6 (3)
C11—N2—C12	117.9 (3)	C15—C16—H16	120.2
C11—N2—Mn1	125.9 (2)	C17—C16—H16	120.2
C12—N2—Mn1	116.0 (2)	C16—C17—C13	117.6 (3)
C14—N3—C13	117.9 (3)	C16—C17—C18	123.3 (3)
C14—N3—Mn1	126.2 (2)	C13—C17—C18	119.1 (3)

## supplementary materials

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C13—N3—Mn1	115.8 (2)	C19—C18—C17	121.3 (3)
C23—N4—C24	117.7 (3)	C19—C18—H18	119.3
C23—N4—Mn1	126.4 (2)	C17—C18—H18	119.3
C24—N4—Mn1	115.8 (2)	C18—C19—C20	121.0 (3)
N1—C1—C5	123.3 (3)	C18—C19—H19	119.5
N1—C1—C12	117.9 (3)	C20—C19—H19	119.5
C5—C1—C12	118.7 (3)	C21—C20—C24	117.9 (3)
N1—C2—C3	123.3 (4)	C21—C20—C19	123.0 (3)
N1—C2—H2	118.4	C24—C20—C19	119.1 (3)
C3—C2—H2	118.4	C22—C21—C20	119.7 (3)
C4—C3—C2	119.5 (4)	C22—C21—H21	120.2
C4—C3—H3	120.3	C20—C21—H21	120.2
C2—C3—H3	120.3	C21—C22—C23	118.9 (3)
C3—C4—C5	119.2 (3)	C21—C22—H22	120.6
C3—C4—H4	120.4	C23—C22—H22	120.6
C5—C4—H4	120.4	N4—C23—C22	123.5 (3)
C1—C5—C4	117.0 (3)	N4—C23—H23	118.2
C1—C5—C6	119.8 (4)	C22—C23—H23	118.2
C4—C5—C6	123.1 (3)	N4—C24—C20	122.3 (3)
C7—C6—C5	121.4 (3)	N4—C24—C13	117.9 (3)
C7—C6—H6	119.3	C20—C24—C13	119.8 (3)
C5—C6—H6	119.3	O2—C25—O1	131.3 (3)
C6—C7—C8	120.3 (4)	O2—C25—C26	116.1 (3)
C6—C7—H7	119.9	O1—C25—C26	112.5 (3)
C8—C7—H7	119.9	F1—C26—F2	106.1 (3)
C12—C8—C9	117.8 (3)	F1—C26—C25	112.2 (3)
C12—C8—C7	119.5 (3)	F2—C26—C25	111.7 (3)
C9—C8—C7	122.7 (3)	F1—C26—C12	108.6 (3)
C10—C9—C8	119.5 (4)	F2—C26—C12	107.7 (2)
C10—C9—H9	120.3	C25—C26—C12	110.3 (3)
C8—C9—H9	120.3		
N2—Mn1—O1—C25	-45.9 (3)	C12—C8—C9—C10	1.0 (5)
N1—Mn1—O1—C25	24.8 (3)	C7—C8—C9—C10	-178.5 (3)
N4—Mn1—O1—C25	-121.0 (3)	C8—C9—C10—C11	-1.4 (5)
N3—Mn1—O1—C25	-139.1 (3)	C12—N2—C11—C10	0.9 (5)
C11—Mn1—O1—C25	119.4 (3)	Mn1—N2—C11—C10	-175.2 (2)
O1—Mn1—N1—C2	96.7 (3)	C9—C10—C11—N2	0.4 (5)
N2—Mn1—N1—C2	178.0 (3)	C11—N2—C12—C8	-1.3 (5)
N4—Mn1—N1—C2	-97.7 (3)	Mn1—N2—C12—C8	175.2 (2)
N3—Mn1—N1—C2	-135.8 (3)	C11—N2—C12—C1	177.6 (3)
C11—Mn1—N1—C2	-5.3 (3)	Mn1—N2—C12—C1	-5.9 (4)
O1—Mn1—N1—C1	-87.0 (2)	C9—C8—C12—N2	0.4 (5)
N2—Mn1—N1—C1	-5.7 (2)	C7—C8—C12—N2	179.9 (3)
N4—Mn1—N1—C1	78.7 (2)	C9—C8—C12—C1	-178.5 (3)
N3—Mn1—N1—C1	40.5 (4)	C7—C8—C12—C1	1.0 (5)
C11—Mn1—N1—C1	171.1 (2)	N1—C1—C12—N2	0.7 (4)
O1—Mn1—N2—C11	-66.0 (3)	C5—C1—C12—N2	-179.0 (3)
N1—Mn1—N2—C11	-177.7 (3)	N1—C1—C12—C8	179.7 (3)
N4—Mn1—N2—C11	88.6 (3)	C5—C1—C12—C8	0.0 (5)



N3—Mn1—N2—C11	16.7 (3)	C14—N3—C13—C17	-1.5 (5)
Cl1—Mn1—N2—C11	171.2 (2)	Mn1—N3—C13—C17	174.8 (3)
O1—Mn1—N2—C12	117.8 (2)	C14—N3—C13—C24	178.3 (3)
N1—Mn1—N2—C12	6.1 (2)	Mn1—N3—C13—C24	-5.3 (4)
N4—Mn1—N2—C12	-87.6 (2)	C13—N3—C14—C15	0.8 (5)
N3—Mn1—N2—C12	-159.4 (2)	Mn1—N3—C14—C15	-175.1 (3)
Cl1—Mn1—N2—C12	-5.0 (4)	N3—C14—C15—C16	0.3 (6)
O1—Mn1—N3—C14	-6.1 (3)	C14—C15—C16—C17	-0.8 (6)
N2—Mn1—N3—C14	-93.8 (3)	C15—C16—C17—C13	0.1 (5)
N1—Mn1—N3—C14	-137.4 (3)	C15—C16—C17—C18	179.2 (4)
N4—Mn1—N3—C14	-177.8 (3)	N3—C13—C17—C16	1.1 (5)
Cl1—Mn1—N3—C14	93.7 (3)	C24—C13—C17—C16	-178.8 (3)
O1—Mn1—N3—C13	177.9 (2)	N3—C13—C17—C18	-178.1 (3)
N2—Mn1—N3—C13	90.2 (2)	C24—C13—C17—C18	2.1 (5)
N1—Mn1—N3—C13	46.6 (4)	C16—C17—C18—C19	179.0 (4)
N4—Mn1—N3—C13	6.1 (2)	C13—C17—C18—C19	-1.9 (6)
Cl1—Mn1—N3—C13	-82.3 (2)	C17—C18—C19—C20	0.0 (6)
O1—Mn1—N4—C23	159.6 (3)	C18—C19—C20—C21	-178.0 (4)
N2—Mn1—N4—C23	83.7 (3)	C18—C19—C20—C24	1.7 (5)
N1—Mn1—N4—C23	11.4 (3)	C24—C20—C21—C22	0.2 (5)
N3—Mn1—N4—C23	178.4 (3)	C19—C20—C21—C22	179.9 (4)
Cl1—Mn1—N4—C23	-79.1 (3)	C20—C21—C22—C23	1.0 (6)
O1—Mn1—N4—C24	-25.2 (4)	C24—N4—C23—C22	-0.3 (5)
N2—Mn1—N4—C24	-101.0 (2)	Mn1—N4—C23—C22	174.8 (3)
N1—Mn1—N4—C24	-173.4 (2)	C21—C22—C23—N4	-1.0 (6)
N3—Mn1—N4—C24	-6.4 (2)	C23—N4—C24—C20	1.6 (5)
Cl1—Mn1—N4—C24	96.1 (2)	Mn1—N4—C24—C20	-174.1 (3)
C2—N1—C1—C5	1.2 (5)	C23—N4—C24—C13	-178.2 (3)
Mn1—N1—C1—C5	-175.5 (2)	Mn1—N4—C24—C13	6.1 (4)
C2—N1—C1—C12	-178.5 (3)	C21—C20—C24—N4	-1.5 (5)
Mn1—N1—C1—C12	4.8 (4)	C19—C20—C24—N4	178.8 (3)
C1—N1—C2—C3	0.7 (5)	C21—C20—C24—C13	178.3 (3)
Mn1—N1—C2—C3	176.9 (3)	C19—C20—C24—C13	-1.4 (5)
N1—C2—C3—C4	-1.8 (5)	N3—C13—C24—N4	-0.5 (5)
C2—C3—C4—C5	1.0 (5)	C17—C13—C24—N4	179.3 (3)
N1—C1—C5—C4	-1.8 (5)	N3—C13—C24—C20	179.7 (3)
C12—C1—C5—C4	177.9 (3)	C17—C13—C24—C20	-0.5 (5)
N1—C1—C5—C6	180.0 (3)	Mn1—O1—C25—O2	-18.7 (6)
C12—C1—C5—C6	-0.3 (5)	Mn1—O1—C25—C26	161.9 (2)
C3—C4—C5—C1	0.7 (5)	O2—C25—C26—F1	-14.5 (5)
C3—C4—C5—C6	178.8 (3)	O1—C25—C26—F1	164.9 (3)
C1—C5—C6—C7	-0.2 (5)	O2—C25—C26—F2	-133.6 (3)
C4—C5—C6—C7	-178.3 (3)	O1—C25—C26—F2	45.9 (4)
C5—C6—C7—C8	1.2 (5)	O2—C25—C26—Cl2	106.7 (3)
C6—C7—C8—C12	-1.6 (5)	O1—C25—C26—Cl2	-73.8 (3)
C6—C7—C8—C9	177.9 (3)		

Fig. 1

