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Bis[nitratobis(pentafluorobenzoato)-(1,10-phenanthroline-κ^2N,N')manganese(II)] dinitratobis(1,10-phenanthroline-κ^2N,N')manganese(II)

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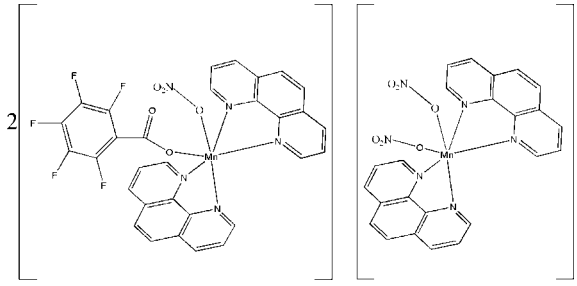
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.097; data-to-parameter ratio = 12.8.

The title compound, $[Mn(C_7F_5O_2)(NO_3)(C_{12}H_8N_2)_2]_2\cdot[Mn(NO_3)_2(C_{12}H_8N_2)_2]$, contains two types of molecules: $[Mn(phen)_2(F_5C_6COO)(NO_3)]$ (A) and $[Mn(phen)_2(NO_3)_2]$ (B) (phen = 1,10-phenanthroline) in a 2:1 ratio. Molecule B possesses a crystallographically imposed twofold rotation axis. The Mn ions in each of the two molecules are coordinated by four N atoms and two O atoms in a distorted octahedral geometry. The crystal packing exhibits $\pi\cdots\pi$ interactions with relatively short distances of 3.6775 (14) and 3.8214 (13) Å between the centroids of six-membered rings from neighbouring molecules, and weak intermolecular C—H$\cdots$O and C—H$\cdots$F hydrogen bonds.

Related literature

Fluorobenzene derivatives such as pentafluorobenzoic acid have been studied by single-crystal X-ray structure analysis (Benghiat & Leiserowitz, 1972; Bach *et al.*, 2001). $C_6F_5CO_2H$, $C_6F_4HCO_2H$ or monofluorobenzoic acid derivatives have been used to prepare metal carboxylates (Mitsuhiro *et al.*, 2003; Ribas *et al.*, 1997). For an attractive interaction between the F atom of fluorobenzene and a π system, see: Thalladi *et al.* (1998).



Experimental

Crystal data

$[Mn(C_7F_5O_2)(NO_3)(C_{12}H_8N_2)_2]_2\cdot[Mn(NO_3)_2(C_{12}H_8N_2)_2]$
M_r = 1916.22
Monoclinic, $C2/c$
a = 45.889 (3) Å
b = 10.1112 (6) Å
c = 17.7948 (10) Å
β = 110.756 (1)°
V = 7720.8 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 295 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.911, T_{max} = 0.933
21136 measured reflections
7585 independent reflections
6126 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.02
7585 reflections
591 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O2	2.1111 (15)	Mn1—N2	2.3202 (18)
Mn1—O3	2.2073 (16)	Mn2—O7	2.1988 (19)
Mn1—N3	2.2405 (18)	Mn2—N6	2.2808 (18)
Mn1—N4	2.2708 (18)	Mn2—N7	2.3124 (18)
Mn1—N1	2.3034 (18)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C9—H9$\cdots$O3^{i}	0.93	2.56	3.474 (3)	170
C9—H9$\cdots$O5^{i}	0.93	2.57	3.221 (3)	127
C13—H13$\cdots$O5^{ii}	0.93	2.59	3.485 (3)	162
C24—H24$\cdots$O6^{iii}	0.93	2.59	3.220 (4)	125
C27—H27$\cdots$O2^{iii}	0.93	2.54	3.455 (3)	170
C39—H39$\cdots$O1^{iv}	0.93	2.54	3.306 (4)	139
C43—H43$\cdots$O8^{v}	0.93	2.56	3.412 (3)	153
C28—H28$\cdots$F1^{iii}	0.93	2.61	3.288 (3)	131
C33—H33$\cdots$F5^{vi}	0.93	2.58	2.915 (3)	101

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

Table 3
$\pi\cdots\pi$ interactions (Å).

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the rings N7/C38–C42, C35–C37/C41–C43, C2–C7 and C11–C14/C18/C19, respectively.

*Cg*1—*Cg*2^{vii}	3.6775 (14)	*Cg*3—*Cg*4^{viii}	3.8214 (13)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: Bruker *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2276).

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supplementary materials

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Bis[nitratobis(pentafluorobenzoato)(1,10-phenanthroline-κ^2N,N')manganese(II)] dinitrato-bis(1,10-phenanthroline-κ^2N,N')manganese(II)

X. Zhang, C. Ge, X. Zhang, Y. Guo and Q. Liu

Comment

The title compound contains two types of neutral molecules - $Mn(Phen)_2(F_5C_6COO)(NO_3)$ (A) and $Mn(Phen)_2(NO_3)_2$ (B), respectively, with a 2:1 ratio. The Mn ions in two molecules are coordinated by four N atoms and two O atoms in a distorted octahedral geometry each (Table 2).

In the crystal, significant F···F interactions are favored (F3···F3($1/2-x$,$-1/2-y$,$1-z$) = 2.813 (2) Å; F3—F4($1/2-x$,$-1/2-y$,$1-z$) =3.020 (3) Å). The crystal packing exhibits weak intermolecular C—H···O and C—H···F hydrogen bonds (Table 1), and π···π interactions proved by relatively short distances of 3.6775 (14) and 3.8214 (13) Å between the centroids of six-membered rings from the neighbouring molecules (Table 2).

Experimental

The title compound was obtained as following: added aqueous solution of manganese(II) nitrate (1 mmol) and phen (3 mmol) slowly to aqueous solution of pentafluorobenzoic acid (1 mmol) and KOH (1 mmol) with stirring, then the resulting mixture was stirred 4 h under refluxing. The solution was filtered. By slow evaporation, yellow block-shape single crystals suitable for X-ray analysis were obtained within several weeks.

Refinement

All H atoms were geometrically positioned [C—H 0.93 Å], and treated as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

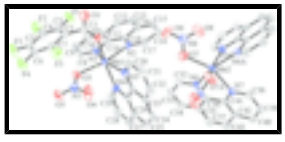


Fig. 1. View of (I), showing atomic labels and displacement ellipsoids drawn at the 50% probability level [symmetry code: (A) $-x$, y, $-z+1/2$]. H atoms omitted for clarity.

Bis[bis(1,10-phenanthroline-κ^2N,N')\ (pentafluorobenzenecarboxylato)nitratomanganese(II)] [bis(1,10-phenanthroline-κ^2N,N')dinitratomanganese(II)]

Crystal data

$[Mn(C_7F_5O_2)(NO_3)(C_{12}H_8N_2)_2]_2\cdot[Mn(NO_3)_2(C_{12}H_8N_2)_2]$	$Z = 4$
$M_r = 1916.22$	$D_x = 1.649$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation

	λ = 0.71073 Å
Hall symbol: -C2yc	Cell parameters from 749 reflections
a = 45.889 (3) Å	θ = 2.6–22.7º
b = 10.1112 (6) Å	μ = 0.59 mm^{-1}
c = 17.7948 (10) Å	T = 295 (2) K
β = 110.7560 (10)º	Block, yellow
V = 7720.8 (8) Å^3	0.15 × 0.12 × 0.10 mm
Z = 4	

Data collection

CCD area-detector diffractometer	7585 independent reflections
Radiation source: fine-focus sealed tube	6126 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 293(2) K	θ_{max} = 26.1º
phi and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -52 \rightarrow 56$
T_{min} = 0.911, T_{max} = 0.933	$k = -11 \rightarrow 12$
21136 measured reflections	$l = -19 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained
$wR(F^2)$ = 0.097	$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 5.7994P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
7585 reflections	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
591 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C43	0.03336 (6)	1.1563 (2)	0.50464 (15)	0.0444 (6)
H43	0.0310	1.2245	0.5371	0.053*
C42	0.00697 (6)	1.1132 (2)	0.43748 (13)	0.0350 (5)
Mn1	0.148454 (7)	0.35412 (3)	0.382044 (19)	0.02757 (10)
N5	0.16267 (4)	0.14679 (19)	0.50756 (12)	0.0356 (4)
O3	0.17706 (4)	0.20487 (16)	0.46679 (9)	0.0402 (4)
F1	0.20011 (3)	0.17676 (16)	0.25519 (10)	0.0578 (4)
F3	0.24872 (4)	−0.14013 (16)	0.45045 (10)	0.0661 (5)
F4	0.19236 (4)	−0.21137 (16)	0.45704 (10)	0.0672 (5)
O5	0.17547 (4)	0.05628 (17)	0.55339 (10)	0.0480 (4)
O2	0.13379 (4)	0.22998 (16)	0.28005 (9)	0.0380 (4)
N4	0.15013 (4)	0.48379 (18)	0.48769 (10)	0.0311 (4)
N1	0.19547 (4)	0.42421 (18)	0.37690 (11)	0.0321 (4)
F5	0.14027 (4)	−0.08701 (17)	0.36266 (10)	0.0622 (4)
N3	0.09923 (4)	0.37216 (18)	0.37779 (11)	0.0330 (4)
N2	0.13914 (4)	0.53424 (17)	0.29593 (10)	0.0300 (4)
C1	0.13860 (5)	0.1196 (2)	0.25465 (13)	0.0343 (5)
C11	0.22118 (5)	0.5765 (2)	0.31515 (13)	0.0351 (5)
C2	0.16855 (5)	0.0482 (2)	0.30657 (13)	0.0322 (5)
C5	0.22249 (6)	−0.0790 (2)	0.40499 (15)	0.0434 (6)
C31	0.09537 (5)	0.4385 (2)	0.43976 (13)	0.0314 (5)
C4	0.22417 (6)	0.0196 (3)	0.35357 (16)	0.0459 (6)
C23	0.06602 (6)	0.4514 (2)	0.44829 (15)	0.0406 (6)
C19	0.19443 (5)	0.5265 (2)	0.32645 (12)	0.0302 (5)
C14	0.16242 (5)	0.6912 (2)	0.23027 (13)	0.0344 (5)
C30	0.12250 (5)	0.4971 (2)	0.49869 (13)	0.0308 (5)
C15	0.13288 (6)	0.7456 (2)	0.19022 (14)	0.0422 (6)
H15	0.1305	0.8162	0.1551	0.051*
C3	0.19740 (6)	0.0817 (2)	0.30517 (14)	0.0394 (6)
C18	0.16441 (5)	0.5852 (2)	0.28339 (12)	0.0288 (5)
O1	0.12288 (5)	0.06588 (19)	0.19263 (11)	0.0615 (6)
C17	0.11156 (5)	0.5883 (2)	0.25586 (13)	0.0365 (5)
H17	0.0941	0.5534	0.2635	0.044*
C8	0.22307 (5)	0.3704 (2)	0.41628 (15)	0.0400 (6)
H8	0.2239	0.3001	0.4507	0.048*
F2	0.25214 (3)	0.05384 (19)	0.35069 (12)	0.0786 (6)
C7	0.16769 (6)	−0.0508 (2)	0.35868 (14)	0.0390 (6)
C25	0.08929 (7)	0.5742 (3)	0.57119 (17)	0.0528 (8)
H25	0.0872	0.6184	0.6149	0.063*
C6	0.19429 (6)	−0.1149 (2)	0.40790 (14)	0.0427 (6)
C13	0.19028 (6)	0.7384 (2)	0.22008 (14)	0.0408 (6)
H13	0.1890	0.8077	0.1847	0.049*
C28	0.17431 (7)	0.6064 (3)	0.60876 (15)	0.0528 (7)
H28	0.1924	0.6423	0.6455	0.063*
C29	0.17518 (6)	0.5374 (2)	0.54133 (14)	0.0402 (6)

H29	0.1942	0.5290	0.5340	0.048*
O4	0.13659 (4)	0.1855 (2)	0.50111 (15)	0.0706 (7)
C21	0.04466 (6)	0.3249 (3)	0.32733 (18)	0.0506 (7)
H21	0.0278	0.2854	0.2879	0.061*
C24	0.06391 (7)	0.5208 (3)	0.51567 (17)	0.0512 (7)
H24	0.0446	0.5294	0.5215	0.061*
C10	0.24987 (5)	0.5164 (3)	0.35839 (15)	0.0437 (6)
H10	0.2681	0.5466	0.3526	0.052*
C27	0.14646 (7)	0.6202 (2)	0.61980 (15)	0.0517 (7)
H27	0.1455	0.6665	0.6640	0.062*
C26	0.11950 (6)	0.5648 (2)	0.56462 (14)	0.0407 (6)
C22	0.04045 (6)	0.3911 (3)	0.38896 (18)	0.0490 (7)
H22	0.0207	0.3968	0.3921	0.059*
C16	0.10750 (6)	0.6942 (2)	0.20318 (15)	0.0437 (6)
H16	0.0878	0.7295	0.1771	0.052*
C9	0.25084 (5)	0.4131 (3)	0.40909 (16)	0.0464 (6)
H9	0.2696	0.3723	0.4381	0.056*
C12	0.21817 (6)	0.6845 (2)	0.26066 (15)	0.0406 (6)
H12	0.2359	0.7178	0.2533	0.049*
C20	0.07433 (5)	0.3166 (3)	0.32369 (15)	0.0420 (6)
H20	0.0769	0.2700	0.2814	0.050*
Mn2	0.0000	0.80281 (5)	0.2500	0.03132 (13)
N6	0.04381 (4)	0.85364 (18)	0.35662 (10)	0.0313 (4)
O7	0.03107 (5)	0.64739 (19)	0.23530 (11)	0.0595 (5)
N7	−0.01335 (4)	0.96512 (17)	0.32351 (10)	0.0306 (4)
N8	0.02222 (5)	0.5963 (2)	0.16596 (12)	0.0380 (5)
C36	0.04087 (5)	0.9521 (2)	0.40558 (12)	0.0284 (5)
O6	0.03469 (4)	0.49363 (19)	0.15545 (11)	0.0558 (5)
C38	−0.04137 (5)	1.0173 (2)	0.30939 (14)	0.0377 (5)
H38	−0.0580	0.9855	0.2659	0.045*
C41	0.01066 (5)	1.0118 (2)	0.38751 (12)	0.0289 (5)
O8	0.00093 (5)	0.65110 (19)	0.11162 (12)	0.0600 (5)
C39	−0.04727 (6)	1.1173 (2)	0.35620 (15)	0.0429 (6)
H39	−0.0673	1.1501	0.3443	0.051*
C35	0.06611 (5)	0.9952 (2)	0.47287 (13)	0.0344 (5)
C33	0.09753 (5)	0.8308 (2)	0.44203 (14)	0.0387 (6)
H33	0.1164	0.7866	0.4530	0.046*
C34	0.09500 (5)	0.9304 (2)	0.49049 (14)	0.0397 (6)
H34	0.1121	0.9557	0.5348	0.048*
C40	−0.02308 (6)	1.1661 (2)	0.41972 (15)	0.0411 (6)
H40	−0.0264	1.2339	0.4510	0.049*
C32	0.07157 (5)	0.7955 (2)	0.37567 (14)	0.0372 (5)
H32	0.0737	0.7275	0.3428	0.045*
C37	0.06136 (6)	1.0997 (3)	0.52117 (15)	0.0454 (6)
H37	0.0781	1.1293	0.5652	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C43	0.0645 (18)	0.0331 (13)	0.0360 (14)	−0.0094 (12)	0.0181 (13)	−0.0101 (11)
C42	0.0496 (14)	0.0262 (12)	0.0315 (12)	−0.0034 (10)	0.0173 (11)	0.0023 (9)
Mn1	0.02432 (17)	0.03202 (19)	0.02553 (18)	0.00347 (13)	0.00780 (14)	−0.00017 (14)
N5	0.0316 (10)	0.0351 (11)	0.0360 (11)	−0.0004 (8)	0.0070 (9)	0.0012 (9)
O3	0.0455 (10)	0.0439 (10)	0.0354 (9)	0.0075 (8)	0.0195 (8)	0.0093 (7)
F1	0.0483 (9)	0.0644 (10)	0.0637 (10)	0.0076 (7)	0.0233 (8)	0.0350 (8)
F3	0.0537 (10)	0.0632 (11)	0.0679 (11)	0.0216 (8)	0.0049 (8)	0.0263 (9)
F4	0.0812 (12)	0.0574 (10)	0.0641 (11)	0.0053 (9)	0.0272 (9)	0.0313 (9)
O5	0.0457 (10)	0.0475 (11)	0.0469 (10)	0.0054 (8)	0.0116 (8)	0.0192 (9)
O2	0.0412 (9)	0.0375 (9)	0.0308 (8)	0.0103 (7)	0.0073 (7)	−0.0034 (7)
N4	0.0330 (10)	0.0301 (10)	0.0286 (10)	−0.0011 (8)	0.0089 (8)	−0.0003 (8)
N1	0.0291 (10)	0.0373 (11)	0.0285 (10)	0.0060 (8)	0.0085 (8)	0.0065 (8)
F5	0.0506 (9)	0.0743 (11)	0.0693 (11)	−0.0065 (8)	0.0304 (8)	0.0169 (9)
N3	0.0292 (10)	0.0359 (11)	0.0325 (10)	0.0018 (8)	0.0092 (8)	−0.0002 (8)
N2	0.0295 (10)	0.0309 (10)	0.0273 (9)	0.0054 (8)	0.0072 (8)	−0.0004 (8)
C1	0.0360 (13)	0.0359 (13)	0.0301 (12)	0.0048 (10)	0.0104 (10)	0.0006 (10)
C11	0.0359 (12)	0.0376 (13)	0.0334 (12)	−0.0011 (10)	0.0143 (10)	0.0005 (10)
C2	0.0373 (12)	0.0313 (12)	0.0278 (11)	0.0031 (9)	0.0112 (10)	−0.0024 (9)
C5	0.0393 (14)	0.0418 (14)	0.0439 (14)	0.0129 (11)	0.0081 (12)	0.0099 (12)
C31	0.0337 (12)	0.0283 (12)	0.0355 (12)	0.0085 (9)	0.0162 (10)	0.0085 (9)
C4	0.0353 (13)	0.0489 (16)	0.0535 (16)	0.0060 (11)	0.0156 (12)	0.0111 (13)
C23	0.0410 (14)	0.0362 (13)	0.0537 (16)	0.0143 (10)	0.0279 (13)	0.0191 (11)
C19	0.0317 (11)	0.0324 (12)	0.0261 (11)	0.0021 (9)	0.0096 (9)	−0.0016 (9)
C14	0.0434 (13)	0.0289 (12)	0.0282 (12)	0.0011 (10)	0.0096 (10)	−0.0009 (9)
C30	0.0412 (13)	0.0254 (11)	0.0288 (11)	0.0084 (9)	0.0160 (10)	0.0064 (9)
C15	0.0524 (15)	0.0309 (13)	0.0374 (14)	0.0069 (11)	0.0087 (12)	0.0076 (10)
C3	0.0423 (14)	0.0368 (13)	0.0404 (14)	0.0067 (11)	0.0160 (11)	0.0114 (11)
C18	0.0332 (12)	0.0288 (11)	0.0231 (11)	0.0037 (9)	0.0082 (9)	−0.0021 (9)
O1	0.0604 (12)	0.0545 (12)	0.0471 (11)	0.0161 (9)	−0.0088 (9)	−0.0188 (9)
C17	0.0319 (12)	0.0378 (13)	0.0359 (13)	0.0058 (10)	0.0074 (10)	0.0004 (10)
C8	0.0307 (12)	0.0469 (15)	0.0404 (14)	0.0089 (10)	0.0102 (11)	0.0133 (11)
F2	0.0366 (9)	0.0964 (14)	0.1034 (15)	0.0115 (9)	0.0254 (9)	0.0439 (12)
C7	0.0411 (13)	0.0395 (14)	0.0407 (14)	−0.0038 (11)	0.0197 (11)	0.0004 (11)
C25	0.084 (2)	0.0431 (16)	0.0484 (16)	0.0265 (15)	0.0448 (17)	0.0127 (13)
C6	0.0580 (16)	0.0335 (13)	0.0353 (13)	0.0063 (11)	0.0147 (12)	0.0108 (11)
C13	0.0539 (16)	0.0335 (13)	0.0343 (13)	−0.0037 (11)	0.0147 (12)	0.0042 (10)
C28	0.0695 (19)	0.0415 (15)	0.0361 (14)	−0.0066 (13)	0.0049 (13)	−0.0088 (12)
C29	0.0427 (14)	0.0392 (14)	0.0336 (13)	−0.0050 (11)	0.0072 (11)	−0.0028 (11)
O4	0.0381 (11)	0.0547 (12)	0.124 (2)	0.0078 (9)	0.0341 (12)	0.0272 (12)
C21	0.0274 (13)	0.0558 (17)	0.0612 (18)	−0.0029 (11)	0.0064 (13)	0.0067 (14)
C24	0.0591 (17)	0.0503 (16)	0.0605 (18)	0.0258 (14)	0.0413 (16)	0.0223 (14)
C10	0.0313 (13)	0.0544 (16)	0.0478 (15)	−0.0014 (11)	0.0170 (11)	0.0052 (12)
C27	0.087 (2)	0.0359 (15)	0.0313 (14)	0.0082 (14)	0.0200 (14)	−0.0031 (11)
C26	0.0638 (17)	0.0294 (12)	0.0341 (13)	0.0143 (11)	0.0237 (13)	0.0081 (10)

C22	0.0269 (13)	0.0486 (16)	0.075 (2)	0.0094 (11)	0.0216 (13)	0.0240 (14)
C16	0.0406 (14)	0.0396 (14)	0.0417 (14)	0.0113 (11)	0.0031 (11)	0.0058 (11)
C9	0.0276 (12)	0.0595 (17)	0.0502 (16)	0.0083 (11)	0.0113 (11)	0.0133 (13)
C12	0.0441 (14)	0.0401 (14)	0.0416 (14)	−0.0065 (11)	0.0201 (12)	0.0003 (11)
C20	0.0304 (12)	0.0490 (15)	0.0407 (14)	−0.0030 (11)	0.0053 (11)	0.0004 (11)
Mn2	0.0355 (3)	0.0298 (3)	0.0232 (2)	0.000	0.0037 (2)	0.000
N6	0.0331 (10)	0.0339 (10)	0.0242 (9)	0.0018 (8)	0.0070 (8)	−0.0002 (8)
O7	0.0690 (13)	0.0547 (12)	0.0433 (11)	0.0116 (10)	0.0054 (10)	−0.0206 (9)
N7	0.0325 (10)	0.0291 (10)	0.0272 (10)	0.0013 (8)	0.0069 (8)	0.0027 (8)
N8	0.0367 (11)	0.0407 (12)	0.0383 (12)	−0.0083 (9)	0.0154 (10)	−0.0039 (10)
C36	0.0342 (12)	0.0276 (11)	0.0226 (11)	−0.0038 (9)	0.0089 (9)	0.0030 (9)
O6	0.0485 (11)	0.0610 (12)	0.0629 (12)	0.0015 (9)	0.0261 (10)	−0.0249 (10)
C38	0.0345 (13)	0.0400 (13)	0.0352 (13)	0.0024 (10)	0.0083 (10)	0.0050 (11)
C41	0.0356 (12)	0.0260 (11)	0.0251 (11)	−0.0035 (9)	0.0109 (9)	0.0030 (9)
O8	0.0557 (12)	0.0597 (13)	0.0520 (12)	−0.0066 (10)	0.0036 (10)	0.0132 (10)
C39	0.0430 (14)	0.0416 (14)	0.0473 (15)	0.0133 (11)	0.0201 (12)	0.0102 (12)
C35	0.0387 (13)	0.0362 (13)	0.0257 (11)	−0.0110 (10)	0.0081 (10)	0.0016 (10)
C33	0.0313 (12)	0.0459 (15)	0.0367 (13)	0.0023 (10)	0.0096 (11)	0.0144 (11)
C34	0.0341 (13)	0.0469 (15)	0.0306 (12)	−0.0117 (11)	0.0023 (10)	0.0060 (11)
C40	0.0584 (16)	0.0311 (13)	0.0402 (14)	0.0072 (11)	0.0254 (13)	0.0033 (10)
C32	0.0380 (13)	0.0415 (14)	0.0320 (12)	0.0055 (10)	0.0121 (11)	0.0037 (10)
C37	0.0518 (16)	0.0429 (15)	0.0338 (13)	−0.0139 (12)	0.0057 (12)	−0.0099 (11)

Geometric parameters (Å, °)

C43—C37	1.341 (4)	C8—H8	0.9300
C43—C42	1.435 (3)	C7—C6	1.385 (3)
C43—H43	0.9300	C25—C24	1.345 (4)
C42—C41	1.406 (3)	C25—C26	1.435 (4)
C42—C40	1.407 (3)	C25—H25	0.9300
Mn1—O2	2.1111 (15)	C13—C12	1.342 (3)
Mn1—O3	2.2073 (16)	C13—H13	0.9300
Mn1—N3	2.2405 (18)	C28—C27	1.367 (4)
Mn1—N4	2.2708 (18)	C28—C29	1.401 (3)
Mn1—N1	2.3034 (18)	C28—H28	0.9300
Mn1—N2	2.3202 (18)	C29—H29	0.9300
N5—O4	1.225 (2)	C21—C22	1.356 (4)
N5—O5	1.228 (2)	C21—C20	1.388 (3)
N5—O3	1.283 (2)	C21—H21	0.9300
F1—C3	1.345 (3)	C24—H24	0.9300
F3—C5	1.340 (3)	C10—C9	1.370 (3)
F4—C6	1.334 (3)	C10—H10	0.9300
O2—C1	1.253 (3)	C27—C26	1.396 (4)
N4—C29	1.322 (3)	C27—H27	0.9300
N4—C30	1.357 (3)	C22—H22	0.9300
N1—C8	1.327 (3)	C16—H16	0.9300
N1—C19	1.359 (3)	C9—H9	0.9300
F5—C7	1.337 (3)	C12—H12	0.9300
N3—C20	1.330 (3)	C20—H20	0.9300

N3—C31	1.355 (3)	Mn2—O7^{i}	2.1988 (19)
N2—C17	1.330 (3)	Mn2—O7	2.1988 (19)
N2—C18	1.358 (3)	Mn2—N6	2.2808 (18)
C1—O1	1.212 (3)	Mn2—N6^{i}	2.2808 (18)
C1—C2	1.538 (3)	Mn2—N7	2.3124 (18)
C11—C10	1.406 (3)	Mn2—N7^{i}	2.3124 (18)
C11—C19	1.407 (3)	N6—C32	1.333 (3)
C11—C12	1.434 (3)	N6—C36	1.361 (3)
C2—C7	1.374 (3)	O7—N8	1.264 (3)
C2—C3	1.376 (3)	N7—C38	1.329 (3)
C5—C6	1.363 (4)	N7—C41	1.358 (3)
C5—C4	1.374 (3)	N8—O6	1.231 (3)
C31—C23	1.414 (3)	N8—O8	1.236 (3)
C31—C30	1.440 (3)	C36—C35	1.408 (3)
C4—F2	1.347 (3)	C36—C41	1.440 (3)
C4—C3	1.376 (3)	C38—C39	1.396 (3)
C23—C22	1.409 (4)	C38—H38	0.9300
C23—C24	1.422 (4)	C39—C40	1.365 (4)
C19—C18	1.445 (3)	C39—H39	0.9300
C14—C15	1.401 (3)	C35—C34	1.411 (3)
C14—C18	1.410 (3)	C35—C37	1.426 (3)
C14—C13	1.435 (3)	C33—C34	1.358 (3)
C30—C26	1.407 (3)	C33—C32	1.394 (3)
C15—C16	1.367 (3)	C33—H33	0.9300
C15—H15	0.9300	C34—H34	0.9300
C17—C16	1.391 (3)	C40—H40	0.9300
C17—H17	0.9300	C32—H32	0.9300
C8—C9	1.394 (3)	C37—H37	0.9300
C37—C43—C42	120.9 (2)	C12—C13—H13	119.4
C37—C43—H43	119.6	C14—C13—H13	119.4
C42—C43—H43	119.6	C27—C28—C29	119.1 (2)
C41—C42—C40	117.6 (2)	C27—C28—H28	120.5
C41—C42—C43	119.5 (2)	C29—C28—H28	120.5
C40—C42—C43	122.8 (2)	N4—C29—C28	122.7 (2)
O2—Mn1—O3	96.43 (6)	N4—C29—H29	118.6
O2—Mn1—N3	90.51 (6)	C28—C29—H29	118.6
O3—Mn1—N3	115.29 (6)	C22—C21—C20	119.4 (2)
O2—Mn1—N4	164.15 (6)	C22—C21—H21	120.3
O3—Mn1—N4	89.52 (6)	C20—C21—H21	120.3
N3—Mn1—N4	73.68 (6)	C25—C24—C23	121.2 (2)
O2—Mn1—N1	99.58 (6)	C25—C24—H24	119.4
O3—Mn1—N1	84.19 (6)	C23—C24—H24	119.4
N3—Mn1—N1	157.06 (7)	C9—C10—C11	119.7 (2)
N4—Mn1—N1	95.61 (7)	C9—C10—H10	120.1
O2—Mn1—N2	88.34 (6)	C11—C10—H10	120.1
O3—Mn1—N2	156.01 (6)	C28—C27—C26	119.9 (2)
N3—Mn1—N2	88.07 (6)	C28—C27—H27	120.0
N4—Mn1—N2	92.17 (6)	C26—C27—H27	120.0

N1—Mn1—N2	71.83 (6)	C27—C26—C30	117.3 (2)
O4—N5—O5	121.5 (2)	C27—C26—C25	123.8 (2)
O4—N5—O3	118.83 (19)	C30—C26—C25	118.9 (2)
O5—N5—O3	119.69 (19)	C21—C22—C23	120.0 (2)
N5—O3—Mn1	113.47 (13)	C21—C22—H22	120.0
C1—O2—Mn1	142.82 (15)	C23—C22—H22	120.0
C29—N4—C30	118.25 (19)	C15—C16—C17	119.2 (2)
C29—N4—Mn1	126.88 (16)	C15—C16—H16	120.4
C30—N4—Mn1	114.66 (14)	C17—C16—H16	120.4
C8—N1—C19	117.66 (19)	C10—C9—C8	118.6 (2)
C8—N1—Mn1	125.80 (15)	C10—C9—H9	120.7
C19—N1—Mn1	116.49 (13)	C8—C9—H9	120.7
C20—N3—C31	118.1 (2)	C13—C12—C11	121.2 (2)
C20—N3—Mn1	125.98 (16)	C13—C12—H12	119.4
C31—N3—Mn1	115.71 (14)	C11—C12—H12	119.4
C17—N2—C18	117.50 (19)	N3—C20—C21	123.1 (2)
C17—N2—Mn1	126.45 (15)	N3—C20—H20	118.4
C18—N2—Mn1	116.00 (13)	C21—C20—H20	118.4
O1—C1—O2	127.2 (2)	$O7^{i}$—Mn2—O7	88.77 (11)
O1—C1—C2	117.0 (2)	$O7^{i}$—Mn2—N6	118.66 (7)
O2—C1—C2	115.84 (19)	O7—Mn2—N6	80.93 (7)
C10—C11—C19	117.5 (2)	$O7^{i}$—Mn2—$N6^{i}$	80.93 (7)
C10—C11—C12	123.1 (2)	O7—Mn2—$N6^{i}$	118.66 (7)
C19—C11—C12	119.4 (2)	N6—Mn2—$N6^{i}$	153.95 (9)
C7—C2—C3	116.7 (2)	$O7^{i}$—Mn2—N7	97.30 (7)
C7—C2—C1	121.0 (2)	O7—Mn2—N7	152.55 (6)
C3—C2—C1	122.3 (2)	N6—Mn2—N7	72.64 (6)
F3—C5—C6	121.1 (2)	$N6^{i}$—Mn2—N7	88.77 (6)
F3—C5—C4	119.1 (2)	$O7^{i}$—Mn2—$N7^{i}$	152.55 (6)
C6—C5—C4	119.8 (2)	O7—Mn2—$N7^{i}$	97.30 (7)
N3—C31—C23	122.5 (2)	N6—Mn2—$N7^{i}$	88.77 (6)
N3—C31—C30	117.86 (19)	$N6^{i}$—Mn2—$N7^{i}$	72.64 (6)
C23—C31—C30	119.6 (2)	N7—Mn2—$N7^{i}$	89.58 (9)
F2—C4—C5	119.4 (2)	C32—N6—C36	117.54 (19)
F2—C4—C3	120.7 (2)	C32—N6—Mn2	126.40 (15)
C5—C4—C3	119.9 (2)	C36—N6—Mn2	116.05 (14)
C22—C23—C31	116.9 (2)	N8—O7—Mn2	114.23 (15)
C22—C23—C24	123.9 (2)	C38—N7—C41	117.61 (19)
C31—C23—C24	119.2 (2)	C38—N7—Mn2	127.41 (15)
N1—C19—C11	122.7 (2)	C41—N7—Mn2	114.98 (14)
N1—C19—C18	117.82 (19)	O6—N8—O8	122.7 (2)
C11—C19—C18	119.5 (2)	O6—N8—O7	119.1 (2)
C15—C14—C18	117.4 (2)	O8—N8—O7	118.2 (2)
C15—C14—C13	123.4 (2)	N6—C36—C35	122.2 (2)
C18—C14—C13	119.2 (2)	N6—C36—C41	118.01 (18)
N4—C30—C26	122.8 (2)	C35—C36—C41	119.8 (2)

N4—C30—C31	117.73 (19)	N7—C38—C39	123.6 (2)
C26—C30—C31	119.5 (2)	N7—C38—H38	118.2
C16—C15—C14	119.5 (2)	C39—C38—H38	118.2
C16—C15—H15	120.2	N7—C41—C42	122.7 (2)
C14—C15—H15	120.2	N7—C41—C36	118.18 (19)
F1—C3—C2	120.2 (2)	C42—C41—C36	119.11 (19)
F1—C3—C4	117.9 (2)	C40—C39—C38	118.9 (2)
C2—C3—C4	121.9 (2)	C40—C39—H39	120.6
N2—C18—C14	122.8 (2)	C38—C39—H39	120.6
N2—C18—C19	117.76 (19)	C36—C35—C34	118.0 (2)
C14—C18—C19	119.4 (2)	C36—C35—C37	119.1 (2)
N2—C17—C16	123.5 (2)	C34—C35—C37	122.8 (2)
N2—C17—H17	118.2	C34—C33—C32	119.2 (2)
C16—C17—H17	118.2	C34—C33—H33	120.4
N1—C8—C9	123.9 (2)	C32—C33—H33	120.4
N1—C8—H8	118.1	C33—C34—C35	119.3 (2)
C9—C8—H8	118.1	C33—C34—H34	120.4
F5—C7—C2	119.2 (2)	C35—C34—H34	120.4
F5—C7—C6	118.3 (2)	C39—C40—C42	119.6 (2)
C2—C7—C6	122.5 (2)	C39—C40—H40	120.2
C24—C25—C26	121.6 (2)	C42—C40—H40	120.2
C24—C25—H25	119.2	N6—C32—C33	123.7 (2)
C26—C25—H25	119.2	N6—C32—H32	118.1
F4—C6—C5	120.3 (2)	C33—C32—H32	118.1
F4—C6—C7	120.6 (2)	C43—C37—C35	121.5 (2)
C5—C6—C7	119.2 (2)	C43—C37—H37	119.2
C12—C13—C14	121.3 (2)	C35—C37—H37	119.2

Symmetry codes: (i) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O3^{ii}	0.93	2.56	3.474 (3)	170
C9—H9···O5^{ii}	0.93	2.57	3.221 (3)	127
C13—H13···O5^{iii}	0.93	2.59	3.485 (3)	162
C24—H24···O6^{iv}	0.93	2.59	3.220 (4)	125
C27—H27···O2^{iv}	0.93	2.54	3.455 (3)	170
C39—H39···O1^{v}	0.93	2.54	3.306 (4)	139
C43—H43···O8^{vi}	0.93	2.56	3.412 (3)	153
C28—H28···F1^{iv}	0.93	2.61	3.288 (3)	131
C33—H33···F5^{vii}	0.93	2.58	2.915 (3)	101

Symmetry codes: (ii) −*x*+1/2, −*y*+1/2, −*z*+1; (iii) *x*, −*y*+1, *z*−1/2; (iv) *x*, −*y*+1, *z*+1/2; (v) −*x*, *y*+1, −*z*+1/2; (vi) *x*, −*y*+2, *z*+1/2; (vii) *x*, *y*+1, *z*.

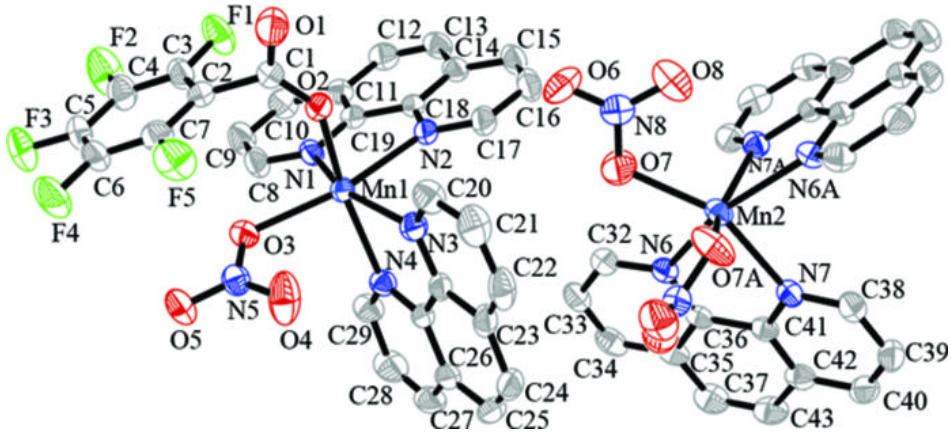
Table 3

π···π interactions (Å)

*Cg*1—*Cg*2^{vii}	3.6775 (14)	*Cg*3—*Cg*4^{viii}	3.8214 (13)

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are centroids of the rings N7/C38–C42, C35–C37/C41–C43, C2–C7 and C11–C14/C18/C19, respectively.
Symmetry codes: (vii) *x*, 2 − *y*, −1/2 + *z*; (viii) *x*, −1 + *y*, *z*.

Fig. 1


F1
O1
F2
C3
C12
C13
C15
C4
C1
C14
O6
O8
C2
O2
C11
C5
C18
C16
N8
F3
C7
C10
C19
N2
C17
C9
N1
Mn1
C20
O7
N7A
N6A
C6
F5
C8
Mn2
F4
C21
O3
N3
C32
N6
C22
N4
O7A
N7
C38
N5
C33
C36
C41
O5
O4
C29
C23
C35
C42
C39
C26
C34
C37
C28
C24
C40
C27
C25
C43