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Supplementary Information

Crystal Structure, Supramolecular Self-Assembly and Interaction with DNA of a Mixed Ligand Manganese(II) Complex

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Table S1. Summary of crystallographic data for complex **1**

Empirical formula	$C_{31}H_{21}ClMnN_4O_6$
Color/shape	Orange/block
Formula weight	635.91
Crystal size / mm	0.40 × 0.29 × 0.21
Temperature / K	298(2)
Crystal system	Monoclinic
Space group	$P2_1/n$
a / Å	16.8160(19)
b / Å	10.6303(15)
c / Å	16.934(2)
β / degree	113.134(2)
V / Å^3	2783.6(6)
Z	4
D_{calc} / (g cm^{-3})	1.517
Absorption coefficient / (mm^{-1})	0.624
Absorption correction	SADABS
Max. and min. transmission	0.8802 and 0.7885
Data/restraints/parameters	4887 / 0 / 388
F(000)	1300
Theta range / degree	1.45 to 25.01
Reflection collected	13646
Independent reflections	4887
Goodness-of-fit on F^2	1.003
R_1, wR_2 [I>2σ (I)]	0.0604, 0.1508
Largest diff. peak and hole / (e Å^{-3})	0.510, –0.360

Table S2. Selected bond lengths (Å) and angles (°) for complex **1**

Mn(1)–O(2)	2.057(4)	Mn(1)–N(4)	2.234(5)
Mn(1)–O(1)	2.158(4)	Mn(1)–N(1)	2.264(4)
Mn(1)–N(3)	2.227(5)	Mn(1)–N(2)	2.346(5)
O(2)–Mn(1)–O(1)	84.12(16)	N(1)–Mn(1)–N(2)	71.69(17)
O(2)–Mn(1)–N(3)	91.89(16)	O(1)–Mn(1)–N(1)	102.47(17)
O(1)–Mn(1)–N(3)	160.36(17)	N(3)–Mn(1)–N(1)	96.62(16)
O(2)–Mn(1)–N(4)	113.54(16)	N(4)–Mn(1)–N(1)	155.92(17)
O(1)–Mn(1)–N(4)	90.1(2)	O(2)–Mn(1)–N(2)	159.07(16)
N(3)–Mn(1)–N(4)	73.81(19)	O(1)–Mn(1)–N(2)	93.76(16)
O(2)–Mn(1)–N(1)	88.39(16)	N(3)–Mn(1)–N(2)	96.62(16)
N(4)–Mn(1)–N(2)	87.24(17)	C(3)–O(2)–Mn(1)	130.9(3)

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Table S3. Data of π-π stacking interactions in complex **1**[a,b,c,d]

Stacking moieties (mode)	h	α	r	θ	d	A	B	C
N4–phen and N4A–phen (I)	3.520	0	1.23	19.32	A′	6.450	4.801	3.849
					B′	4.801	3.995	3.629
					C′	3.849	3.629	4.667
N2–py and N1A–py (II)	3.504	11	1.44	22.29	A′	6.249	4.974	3.787
					B′	7.863	6.845	5.117
					C′	9.978	8.621	6.677
					short contacts			
N3–py and C7A–ar (III)	3.721	17.60	0.98	14.82	C23···C5A: 3.472; C23···C6A: 3.446 C24···C6A: 3.418			
C7–ar and N1A–phen (IV)		95.50			C7···X2: 3.874; H6···C17A: 2.852; H7···X2: 2.970; H7···C13A: 2.887			

[a]Symmetry codes: I 2–x, 2–y,–z; II 1.5–x, 0.5+y, 0.5–z; III 0.5+x, 1.5–y, –0.5+z; IV 0.5+x, 1.5–y, 0.5+z.
[b]N4–phen represents the N4–bound phenanthroline; N2–py represents the N2–bound pyridine moiety of phenanthroline; C7–ar represents the C7–bound arene.
[c]d Centroid-centroid distance (Å); h Interplanar separation (Å); α dihedral angle (°); θ Slip angle (°); r Centroid displacement (Å). $\cos\theta = h/d$; $r^2 = d^2 - h^2$.
[d]A, B, C, A′, B′ and C′ represent the six-membered rings in two stacking phenanthroline ligands. X2 represents the centroid of phenanthroline ligand.

Table S4. A list of hydrogen bonds in complex **1** (Å, °)[a]

D–H···A	D–H	H···A	D···A	∠DHA
C1–H1···O5#1	0.93	2.59	3.22	155
C8–H8···O2	0.93	2.55	3.12	120
C10–H10···O1#2	0.93	2.55	3.32	141
C31–H31···O2#3	0.93	2.53	3.19	128
C22–H22···O3#4	0.93	2.69	3.44	138
C29–H29···O3#5	0.93	2.66	3.38	135

[a]Symmetry codes: #1 0.5–x, 0.5+y, 0.5–z; #2 1.5–x, –0.5+y, 0.5–z; #3 1–x, 1–y, 1–z; #4 1+x, 1+y, z; #5 1–x, 1–y, –z.