Hydrogen Bonding-Driven Structural Modulation in Narrowband Green-Emitting Mn^{2+} Hybrids for Enhanced X-ray Imaging Performance

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Table S1. Crystal data and structure refinement for $[MePi]MnBr_4$.

Formula weight	322.94
Temperature/K	150.00(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	11.48130(10)
b/Å	9.70780(10)
c/Å	23.8200(2)
α/°	90
β/°	90
γ/°	90
Volume/$Å^3$	2654.93(4)
Z	8
$\rho_{calc}g/cm^3$	1.616
μ/mm^{-1}	15.648
F(000)	1307.0
Crystal size/mm^3	0.2 × 0.1 × 0.01
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.422 to 154.462
Index ranges	-12 ≤ h ≤ 14, -12 ≤ k ≤ 12, -29 ≤ l ≤ 30
Reflections collected	26087
Independent reflections	2804 [R_{int} = 0.0598, R_{sigma} = 0.0241]
Data/restraints/parameters	2804/0/119
Goodness-of-fit on F^2	7.321
Final R indexes [I>=2σ (I)]	R_1 = 0.2177, wR_2 = 0.5689
Final R indexes [all data]	R_1 = 0.2195, wR_2 = 0.5707
Largest diff. peak/hole / e $Å^{-3}$	33.04/-3.86

Table S2. Crystal data and structure refinement for $[EtPi]MnBr_4$.

Empirical formula	$C_5H_{14}Br_4MnN_2$
Formula weight	476.76
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.7250(2)
b/Å	15.3816(3)
c/Å	10.1342(2)
α/°	90
β/°	90.423(2)
γ/°	90
Volume/Å^3	1360.02(5)
Z	4
ρ_{calc}g/cm^3	2.328
μ/mm^{-1}	21.354
F(000)	892.0
Crystal size/mm^3	0.05 × 0.02 × 0.01
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	10.454 to 154.918
Index ranges	-10 ≤ h ≤ 10, -19 ≤ k ≤ 19, -12 ≤ l ≤ 10
Reflections collected	13492
Independent reflections	2801 [R_{int} = 0.0472, R_{sigma} = 0.0248]
Data/restraints/parameters	2801/0/110
Goodness-of-fit on F^2	1.229
Final R indexes [I>=2σ (I)]	R_1 = 0.0463, wR_2 = 0.1244
Final R indexes [all data]	R_1 = 0.0470, wR_2 = 0.1249
Largest diff. peak/hole / e Å^{-3}	1.47/-1.85

Table S3. Bond Lengths for [MePi]$MnBr_4$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Mn1	Br1	2.367(4)	N1	C2	1.52(2)
Mn1	Br4	2.350(4)	N2	C6	1.49(2)
Mn1	Br2	2.396(4)	N2	C3	1.50(2)
Mn1	Br3	2.327(4)	C1	C6	1.54(2)
N1	C1	1.50(2)	C4	C3	1.53(3)
N1	C4	1.51(2)	C2	C5	1.51(3)

Table S4. Bond Angles for [MePi]$MnBr_4$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Br1	Mn1	Br2	106.77(16)	C4	N1	C2	109.0(14)
Br4	Mn1	Br1	106.89(15)	C6	N2	C3	111.2(14)
Br4	Mn1	Br2	106.35(15)	N1	C1	C6	110.3(14)
Br3	Mn1	Br1	112.23(16)	N1	C4	C3	110.3(14)
Br3	Mn1	Br4	119.52(17)	N2	C6	C1	110.2(15)
Br3	Mn1	Br2	104.25(15)	N2	C3	C4	109.8(14)
C1	N1	C2	110.8(14)	N1	C2	C5	113.3(16)
C4	N1	C1	112.8(14)				

Table S5. Bond Lengths for [EtPi]$MnBr_4$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	Mn1	2.5179(10)	C5	N5	1.499(7)
Br4	Mn1	2.5090(10)	C5	C3	1.500(6)
Br2	Mn1	2.4980(10)	N3	C4	1.526(7)
Br3	Mn1	2.4786(10)	N3	C3	1.510(7)
C1	N3	1.515(6)	N5	C2	1.503(8)
C1	C2	1.491(6)			

Table S6. Bond Angles for [EtPi]$MnBr_4$.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Br4	Mn1	Br1	103.68(3)	C3	C5	N5	110.7(4)
Br2	Mn1	Br1	105.60(4)	C1	N3	C4	108.0(4)
Br2	Mn1	Br4	108.61(4)	C3	N3	C1	108.6(4)
Br3	Mn1	Br1	110.52(4)	C3	N3	C4	111.2(4)
Br3	Mn1	Br4	115.46(4)	C2	N5	C5	110.1(4)
Br3	Mn1	Br2	112.20(4)	C5	C3	N3	110.4(4)
C2	C1	N3	112.7(4)	C1	C2	N5	109.7(4)