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Electronic supplementary information

Near-Unity and High Anti-Thermal Quenching Red Luminescence from One-Dimensional Hybrid Manganese Chloride for Efficient and Stable White Light-Emitting Diodes

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Table S1. The crystal structure parameters of (TMA)$MnCl_3$

Chemical formula	$C_4H_{12}Cl_3MnN$
Molecular weight	235.44
Temperature (K)	293
Space group, *Z*	$P6_3/m$, 2
a (Å)	9.1504 (6)
c (Å)	6.4984 (4)
V (Å^3)	471.21 (7)
ρ_{calc} (g/cm^3)	1.659
μ (mm^{-1})	2.176
Reflections measured	3710
Reflections independent	445
Reflections with $F > 4\sigma(F)$	393
$2\theta_{max}$ (°)	58.44
R_{int}	0.0623
Number of refinement parameters	21
R_1 [$F_o > 4\sigma(F_o)$][a]	0.0446
wR_2[b]	0.1020
Goof	1.130
$\Delta\rho_{max}$ (e/Å^3)	0.482
$\Delta\rho_{min}$ (e/Å^3)	-0.687
$(\Delta/\sigma)_{max}$	<0.001
Extinction coefficient (SHELXL 2014/7)	1.43 (9)

[a] $R_1 = \sum \| F_o | - | F_c \| / \sum | F_o |$, [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$.

Table S2. The main bond lengths (Å) of (TMA)$MnCl_3$

Mn—Cl	2.5620 (7)	N—C16	1.438 (7)
Mn—Cl1	2.5620 (7)	N—C17	1.438 (7)
Mn—Cl2	2.5620 (7)	N—C18	1.438 (7)
Mn—Cl3	2.5620 (7)	N—C2	1.562 (19)
Mn—Cl4	2.5620 (7)	N—C2	1.562 (19)
Mn—Cl5	2.5620 (7)		

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

Table S3. The main bond angles (˚) of (TMA)$MnCl_3$

Atom	**Atom**	**Atom**	**Angle**
Cl	Mn	Cl1	95.922(19)
Cl2	Mn	Cl3	95.92(2)
Cl4	Mn	Cl5	95.92(2)
Cl	Mn	Cl2	84.078(19)
Cl	Mn	Cl5	84.08(2)
Cl1	Mn	Cl2	180.0
Cl1	Mn	Cl3	84.08(2)
Cl	Mn	Cl4	180.0
Cl4	Mn	Cl3	84.08(2)
Cl1	Mn	Cl4	84.079(19)
Cl1	Mn	Cl5	95.92(2)
Cl2	Mn	Cl4	95.921(19)
Cl3	Mn	Cl5	180.00(3)
Cl	Mn	Cl3	95.92(2)
Cl2	Mn	Cl5	84.08(2)

Table S4. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}	*Occ.*
Mn	1.0000	0.0000	0.5000	0.0284 (4)	1
Cl	0.84992 (11)	0.09811 (12)	0.7500	0.0357 (4)	1
N	0.6667	0.3333	0.2500	0.0318 (11)	1
C1	0.6226 (12)	0.1589 (9)	0.2500	0.150 (5)	1
H1A	0.5020	0.0887	0.2500	0.180*	1
H1B	0.6682	0.1358	0.1294	0.180*	0.25
H1C	0.6682	0.1358	0.3706	0.180*	0.25
C2	0.6667	0.3333	0.010 (3)	0.182 (17)	0.5
H2A	0.6944	0.4431	-0.0396	0.219*	0.5
H2B	0.7488	0.3056	-0.0396	0.219*	0.25
H2C	0.5569	0.2512	-0.0396	0.219*	0.25

Table S5. Hydrogen-bond geometry in the $(C_4H_{12}N)MnCl_3$ structure (Å, °)

D—H	d(D—H)	d(H···A)	∠ D—H···A	D···A	A	Transformation for A atom
C(1)—H(1A)	0.96	2.79	177	3.749(11)	Cl	1-x,-y,-1/2+z
C(2)—H(2A)	0.96	2.84	177	3.7283(2)	Cl	1-y, x-y, -1+z

Table S6. PL lifetimes of the (TMA)$MnCl_3$ SCs under different temperatures

Temperatures (K)	Lifetimes (ms)
80	0.901
100	0.884
120	0.868
140	0.845
160	0.825
180	0.795
200	0.764
220	0.736
240	0.707
260	0.678
280	0.652
300	0.623

Table S7. CIE 1931 color coordinates of fabricated white LED device under various operating currents.

Operating currents (mA)	CIE
20	(0.382, 0.382)
40	(0.381, 0.383)
60	(0.381, 0.383)
80	(0.380, 0.384)
100	(0.379, 0.384)
120	(0.378, 0.384)
160	(0.378, 0.384)
200	(0.377, 0.385)
240	(0.375, 0.385)
280	(0.375, 0.385)