Supporting Information

Thermal Stable Zinc-Based Hybrid Halides with High External Quantum Efficiency as Temperature Detectors

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as a function of temperature.**)** **S15**

Table S1. Crystal data and structure refinement for $(C_9H_{15}N_3)ZnCl_4$ at 293(2) K.

Empirical formula	$(C_9H_{15}N_3)ZnCl_4$
Formula weight	1111.17
Temperature	150.0 K
Crystal system	monoclinic
Space group	$P2_1$
Unit-cell dimensions	a = 10.350(2) Å, α = 90° b = 20.076(4) Å, β = 91.748(7)° c = 20.679(4) Å, γ = 90°
Volume	4294.9(14) Å^3
Z	4
Density (calculated)	1.718 g/cm^3
Absorption coefficient	2.422 mm^{-1}
F (000)	2236
θ range for data collection	1.969 to 24.999°
Index ranges	$-12 \leq h \leq 12$, $-23 \leq k \leq 23$, $-24 \leq l \leq 24$
Reflections collected	60098
Independent reflections	14944 [R_{int} = 0.0754]
Completeness to θ = 25.242°	98.8%
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	14944/37/953
Goodness-of-fit	1.076
Final R indices [$I > 2\sigma$(I)]	R_{obs} = 0.0588, wR_{obs} = 0.1488
R indices [all data]	R_{all} = 0.0774, wR_{all} = 0.1615
Largest diff. peak and hole	0.617 and -0.693 e·Å^{-3}

$R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2]/\Sigma[w(|F_o|^4)]\}^{1/2}$ and $w = 1/[\sigma^2(F_o^2) + (0.0778P)^2 + 2.7836P]$ where $P = (F_o^2 + 2F_c^2)/3$

Table S2. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2×10^3) for $(C_9H_{15}N_3)ZnCl_4$ at 150.0 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Zn(02)	6590(2)	7010(1)	7131(1)	1	36(1)
Zn(03)	10520(2)	7060(1)	486(1)	1	45(1)
Zn(04)	6428(8)	4961(2)	1177(3)	0.69(2)	31(2)
Zn(05)	9662(10)	4966(9)	4533(7)	0.423(17)	33(2)
Zn(06)	4058(10)	7046(6)	3846(5)	0.548(16)	40(2)

Cl(07)	8431(3)	10881(2)	1871(2)	1	40(1)
Cl(08)	5212(3)	10076(2)	2062(2)	1	39(1)
Cl(09)	8071(3)	9064(2)	1560(2)	1	44(1)
Cl(0A)	4436(3)	6829(2)	7023(2)	1	42(1)
Cl(0B)	7819(4)	9776(2)	3245(2)	1	55(1)
Cl(0C)	8326(4)	6903(2)	401(2)	1	47(1)
Cl(0D)	7185(3)	6974(2)	8210(2)	1	46(1)
Cl(0E)	9227(5)	4003(2)	4957(2)	1	66(2)
Cl(0F)	5754(17)	4071(5)	1723(5)	0.70(4)	44(3)
Cl(0G)	5909(3)	4912(2)	120(2)	1	53(1)
Cl(0H)	12005(4)	5151(2)	4652(2)	1	53(1)
Cl(0I)	8722(4)	5128(2)	1292(2)	1	51(1)
Cl(0J)	7258(4)	7948(2)	6683(2)	1	51(1)
Cl(0K)	11183(4)	7901(2)	-114(2)	1	52(1)
Cl(0L)	11535(4)	6092(2)	202(2)	1	49(1)
Cl(0M)	9449(4)	5005(2)	3447(2)	1	57(1)
Cl(0N)	1762(4)	6886(2)	3704(2)	1	59(2)
Cl(0O)	5353(15)	5921(4)	1495(7)	0.63(6)	38(3)
Cl(0P)	8778(5)	5810(3)	4990(3)	1	81(2)
Cl(0Q)	7716(16)	6102(8)	6770(8)	0.56(2)	45(2)
Cl(0R)	11073(4)	7179(3)	1567(2)	1	63(2)
Cl(0S)	4757(8)	7878(3)	3248(4)	0.655(16)	46(2)
Cl(0T)	4664(15)	6184(6)	3328(7)	0.346(13)	48(2)
Cl(0U)	4198(4)	7064(3)	4918(2)	1	84(2)
N(00V)	4753(11)	10229(7)	3618(6)	1	44(3)
N(00W)	12318(13)	5372(8)	3095(6)	1	55(4)
C(00X)	10669(12)	7627(8)	7005(7)	1	37(2)
N(00Y)	11217(12)	10307(8)	270(7)	1	61(4)
C(00Z)	4351(11)	7554(7)	1545(7)	1	39(3)
N(010)	10548(10)	7290(6)	7574(6)	1	37(2)
C(011)	11308(13)	9291(8)	904(7)	1	40(3)
N(012)	11380(11)	9629(6)	1499(6)	1	41(3)
C(013)	4499(12)	7602(6)	375(7)	1	34(3)
C(014)	4333(15)	6225(9)	-779(8)	1	52(4)

C(015)	10558(12)	7597(8)	8189(7)	1	37(2)
C(016)	11338(12)	8679(6)	2178(7)	1	32(3)
C(017)	12234(13)	3352(7)	733(7)	1	46(3)
C(32)	12371(14)	3651(7)	1300(8)	1	48(4)
N(01A)	12542(12)	4711(6)	1893(6)	1	40(3)
C(01C)	7287(14)	7541(8)	4921(7)	1	46(3)
C(01D)	11948(15)	10346(9)	1442(7)	1	56(4)
N(01E)	10718(11)	7282(6)	6479(5)	1	39(3)
N(01F)	4364(13)	7272(8)	936(7)	1	57(4)
C(01G)	10994(14)	6566(7)	6427(7)	1	39(3)
N(01H)	4501(11)	7256(6)	-185(6)	1	37(3)
C(01K)	12370(12)	3741(8)	141(7)	1	42(3)
C(01L)	3721(14)	7246(8)	-1335(8)	1	49(4)
H01N()	3752.33	7481.98	-1755.03	1	59
C(01M)	5354(14)	10541(9)	4221(6)	1	47(4)
N(01N)	4385(14)	9616(7)	4823(7)	1	65(4)
C(01O)	11275(15)	8399(8)	2738(9)	1	57(5)
N(30)	11164(12)	9755(7)	2632(6)	1	50(3)
C(01Q)	4487(12)	8238(8)	1585(7)	1	45(4)
C(01R)	4420(20)	9570(10)	3666(8)	1	63(5)
C(01S)	7494(14)	7239(8)	4326(7)	1	46(4)
N(32)	12540(11)	4698(6)	744(5)	1	40(3)
C(01U)	10699(12)	8314(7)	8196(7)	1	37(2)
C(01V)	11771(14)	6416(8)	5882(8)	1	52(4)
C(01W)	11001(17)	7410(9)	5293(8)	1	57(5)
C(01X)	7310(15)	8240(10)	4986(9)	1	61(4)
C(01Z)	10130(15)	7550(9)	5853(7)	1	55(4)
N(020)	7832(13)	8286(7)	3856(6)	1	57(4)
C(021)	11305(11)	9356(9)	2086(7)	1	42(4)
C(022)	4619(12)	8279(7)	435(7)	1	37(3)
C(023)	4989(14)	6612(7)	-271(6)	1	39(3)
C(025)	11063(15)	8778(8)	3298(8)	1	52(4)
C(026)	4502(19)	10384(10)	4822(8)	1	69(5)
C(027)	10731(12)	8311(7)	7047(7)	1	37(2)

N(029)	4323(9)	6585(5)	-1395(5)	1	28(2)
C(02A)	10591(14)	9676(8)	383(7)	1	42(3)
C(02B)	3710(20)	9386(11)	4245(8)	1	80(6)
C(02C)	11195(14)	10739(8)	884(6)	1	39(3)
C(02D)	12513(12)	4365(8)	187(6)	1	41(3)
C(0)	12380(20)	4350(11)	2479(10)	0.53(2)	31(4)
C(02F)	4596(12)	8603(8)	1043(7)	1	42(4)
C(02H)	7596(15)	8604(9)	4435(7)	1	59(4)
C(02I)	12110(20)	5443(9)	1883(8)	1	73(6)
C(02J)	10772(12)	8651(8)	7628(6)	1	37(2)
N(02L)	11214(12)	6643(6)	5269(6)	1	46(3)
C02N()	4395(18)	7644(9)	-831(8)	1	59(4)
C(02O)	10986(17)	9458(10)	3219(8)	1	64(5)
C(02Q)	12525(13)	4373(8)	1315(7)	1	41(3)
C(2B)	12510(30)	4635(13)	3051(14)	0.52(3)	29(5)
C(4)	13260(20)	4502(12)	2480(11)	0.47(2)	31(4)
C(1)	11610(30)	5620(15)	2454(12)	0.376(18)	27(3)
Cl(1)	5780(40)	5825(13)	1740(30)	0.40(6)	63(10)
Zn(8)	7396(2)	9915(1)	2165(1)	1	33(1)
Zn(2)	6792(13)	4936(6)	1270(6)	0.29(2)	31(2)
Zn(1)	3639(10)	7021(8)	3820(7)	0.425(15)	40(2)
Zn(0A)	10053(11)	4955(6)	4514(5)	0.540(17)	33(2)
Cl(1A)	4278(16)	7974(7)	3409(8)	0.333(14)	46(2)
Cl(2A)	7550(20)	6194(10)	6561(9)	0.47(2)	45(2)
Cl(2)	6180(30)	3979(12)	1708(13)	0.30(4)	44(3)
Cl(3)	5074(8)	6095(3)	3553(4)	0.643(14)	48(2)
C(3AA)	3821(14)	9382(10)	6498(8)	1	54(4)
C(1AA)	3896(13)	8739(8)	6583(7)	1	45(3)
C(0AA)	4027(14)	8357(8)	6047(9)	1	57(4)
N(0AA)	4153(13)	8639(8)	5475(8)	1	76(5)
C(5)	3951(12)	9690(8)	5959(6)	1	37(3)
C(6)	4100(13)	9344(9)	5416(7)	1	49(3)
N(1)	8107(10)	6696(5)	1967(5)	1	31(2)
N(2AA)	8014(13)	7315(6)	3205(5)	1	44(3)

C(3)	7786(14)	7600(7)	3791(7)	1	45(3)
C(5AA)	8090(30)	7747(13)	2610(12)	0.57(2)	51(5)
C(4AA)	7690(20)	7449(10)	2043(9)	1	87(8)
C(6AA)	8030(40)	6297(14)	2580(13)	0.57(3)	64(4)
C(7)	8317(19)	6658(7)	3113(8)	1	64(4)
C(8)	8850(50)	6520(16)	2558(15)	0.47(3)	64(4)
C(9)	7210(40)	7660(16)	2592(15)	0.45(2)	51(5)
C(10)	12562(17)	5796(9)	2462(7)	0.624(18)	27(3)
C(2A)	13140(30)	4746(13)	2994(13)	0.48(3)	29(5)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Anisotropic displacement parameters ($Å^2×10^3$) for $(C_9H_{15}N_3)ZnCl_4$ at 150.0 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(02)	33(1)	36(1)	39(1)	-1(1)	3(1)	0(1)
Zn(03)	61(1)	37(1)	36(1)	5(1)	0(1)	-1(1)
Zn(04)	39(3)	31(1)	23(2)	7(2)	-8(2)	3(1)
Zn(05)	34(4)	29(1)	37(2)	-3(4)	6(3)	0(1)
Zn(06)	45(4)	40(2)	34(2)	5(4)	-5(3)	-2(1)
Cl(07)	38(2)	38(2)	45(2)	-7(2)	10(2)	-2(2)
Cl(08)	30(2)	46(2)	40(2)	-3(2)	1(2)	-4(2)
Cl(09)	45(2)	37(2)	51(2)	2(2)	6(2)	-8(2)
Cl(0A)	33(2)	55(2)	38(2)	-2(2)	-2(2)	0(2)
Cl(0B)	57(2)	76(3)	34(2)	-4(2)	0(2)	7(2)
Cl(0C)	63(2)	43(2)	36(2)	2(2)	-1(2)	-2(2)
Cl(0D)	37(2)	53(2)	47(2)	4(2)	-6(2)	8(2)
Cl(0E)	96(3)	43(2)	58(2)	-17(2)	-4(2)	9(2)
Cl(0F)	47(7)	32(3)	52(2)	-1(4)	-17(4)	13(2)
Cl(0G)	48(2)	73(2)	38(2)	13(2)	4(2)	7(2)
Cl(0H)	84(2)	40(2)	36(2)	0(2)	-5(2)	0(2)
Cl(0I)	70(2)	47(2)	36(2)	-2(2)	2(2)	6(2)
Cl(0J)	50(2)	43(2)	60(2)	-6(2)	11(2)	6(2)
Cl(0K)	71(2)	39(2)	47(2)	-5(2)	-1(2)	-1(2)
Cl(0L)	64(2)	36(2)	47(2)	5(2)	11(2)	5(2)
Cl(0M)	78(2)	53(2)	39(2)	-6(2)	-14(2)	4(2)
Cl(0N)	99(3)	41(2)	37(2)	12(2)	9(2)	-1(2)
Cl(0O)	43(4)	38(3)	31(5)	5(3)	-2(4)	0(3)

Cl(0P)	68(3)	72(3)	104(4)	-18(2)	24(2)	-38(3)
Cl(0Q)	47(4)	34(5)	55(8)	12(3)	7(5)	1(5)
Cl(0R)	65(2)	87(3)	37(2)	17(2)	-16(2)	-5(2)
Cl(0S)	56(5)	34(3)	47(4)	4(3)	2(3)	-1(2)
Cl(0T)	69(5)	33(3)	42(4)	6(3)	12(3)	11(3)
Cl(0U)	70(3)	138(5)	43(2)	44(3)	0(2)	8(3)
N(00V)	36(6)	62(9)	35(6)	-4(5)	-1(4)	-13(6)
N(00W)	54(7)	81(10)	29(6)	15(7)	-8(5)	12(6)
C(00X)	38(2)	38(3)	34(2)	9(2)	-6(2)	-2(2)
N(00Y)	42(7)	92(11)	51(8)	-10(7)	4(5)	-23(7)
C(00Z)	31(6)	37(7)	49(8)	-3(5)	-2(5)	-13(6)
N(010)	38(2)	38(3)	34(2)	9(2)	-6(2)	-2(2)
C(011)	43(7)	38(7)	40(7)	-6(5)	5(5)	-6(6)
N(012)	37(6)	44(7)	42(7)	-10(5)	4(5)	-9(5)
C(013)	37(6)	21(6)	44(7)	-6(5)	3(5)	-18(5)
C(014)	50(8)	45(9)	61(10)	12(7)	9(7)	1(8)
C(015)	38(2)	38(3)	34(2)	9(2)	-6(2)	-2(2)
C(016)	36(6)	15(6)	46(8)	8(5)	-9(5)	1(5)
C(017)	60(8)	25(6)	53(8)	1(6)	12(6)	-13(6)
C(32)	66(9)	25(6)	54(8)	0(6)	22(7)	15(5)
N(01A)	63(7)	26(6)	30(6)	14(5)	0(5)	-4(4)
C(01C)	68(9)	41(8)	30(7)	-9(6)	0(6)	8(6)
C(01D)	56(8)	69(10)	41(8)	-32(7)	-16(6)	15(7)
N(01E)	45(6)	50(7)	22(5)	6(5)	8(4)	6(5)
N(01F)	55(7)	46(8)	68(10)	-3(6)	-2(6)	0(7)
C(01G)	59(8)	27(7)	32(7)	24(6)	-9(6)	10(5)
N(01H)	52(6)	24(5)	35(6)	0(4)	11(5)	7(4)
C(01K)	43(7)	46(8)	39(7)	13(6)	8(5)	-8(6)
C(01L)	47(8)	49(9)	51(9)	8(6)	-13(6)	5(7)
C(01M)	56(8)	60(9)	26(6)	-18(7)	2(5)	11(6)
N(01N)	93(10)	46(7)	57(8)	-52(7)	19(7)	-9(6)
C(01O)	64(9)	29(7)	77(12)	5(6)	-30(8)	5(8)
N(30)	58(7)	40(7)	52(8)	6(5)	-10(5)	9(6)
C(01Q)	29(6)	61(10)	45(8)	-15(6)	-4(5)	-16(7)
C(01R)	93(13)	57(11)	38(9)	-36(9)	2(8)	7(8)
C(01S)	67(9)	30(7)	43(8)	-1(6)	8(6)	5(6)
N(32)	51(6)	42(6)	27(5)	-9(5)	-3(4)	0(4)
C(01U)	38(2)	38(3)	34(2)	9(2)	-6(2)	-2(2)

C(01V)	48(8)	46(8)	60(9)	17(6)	-8(6)	-5(7)
C(01W)	61(9)	67(11)	44(9)	28(8)	2(7)	14(8)
C(01X)	58(9)	68(11)	56(10)	7(8)	-2(7)	-6(8)
C(01Z)	64(9)	60(10)	40(8)	32(7)	-3(6)	16(7)
N(020)	89(9)	53(8)	30(6)	-12(7)	4(6)	-11(6)
C(021)	24(6)	71(10)	32(7)	-3(6)	0(5)	-18(7)
C(022)	29(6)	39(8)	44(8)	-6(5)	8(5)	-12(6)
C(023)	51(7)	32(7)	33(7)	7(5)	-9(5)	3(5)
C(025)	68(9)	47(8)	41(8)	-13(7)	-6(7)	7(7)
C(026)	100(13)	73(12)	36(8)	-17(10)	19(8)	3(8)
C(027)	38(2)	38(3)	34(2)	9(2)	-6(2)	-2(2)
N(029)	34(5)	19(5)	31(5)	4(4)	9(4)	-12(4)
C(02A)	52(7)	44(8)	32(7)	-11(6)	12(5)	-10(6)
C(02B)	104(14)	90(14)	47(9)	-59(11)	20(8)	-1(9)
C(02C)	49(7)	41(8)	26(6)	-1(6)	1(5)	-1(5)
C(02D)	40(7)	56(8)	29(6)	0(6)	13(5)	11(6)
C(0)	41(9)	23(8)	30(8)	-3(7)	-2(8)	-5(7)
C(02F)	29(6)	50(9)	47(8)	-1(5)	-2(5)	-17(7)
C(02H)	73(10)	62(10)	42(8)	-10(8)	6(7)	-15(7)
C(02I)	133(17)	46(9)	38(9)	-3(10)	-4(9)	-14(7)
C(02J)	38(2)	38(3)	34(2)	9(2)	-6(2)	-2(2)
N(02L)	69(8)	28(6)	40(7)	23(5)	4(5)	-17(5)
C02N()	83(11)	45(9)	47(9)	6(8)	8(7)	6(7)
C(02O)	80(11)	78(12)	33(8)	-8(9)	-8(7)	-12(8)
C(02Q)	40(7)	44(7)	40(7)	5(5)	8(5)	8(5)
C(2B)	38(14)	21(9)	28(8)	3(10)	3(11)	8(7)
C(4)	41(9)	23(8)	30(8)	-3(7)	-2(8)	-5(7)
C(1)	45(8)	28(8)	8(6)	-5(6)	-4(6)	1(5)
Cl(1)	60(13)	54(7)	76(19)	-13(8)	30(14)	-18(10)
Zn(8)	34(1)	34(1)	31(1)	-4(1)	3(1)	-1(1)
Zn(2)	39(3)	31(1)	23(2)	7(2)	-8(2)	3(1)
Zn(1)	45(4)	40(2)	34(2)	5(4)	-5(3)	-2(1)
Zn(0A)	34(4)	29(1)	37(2)	-3(4)	6(3)	0(1)
Cl(1A)	56(5)	34(3)	47(4)	4(3)	2(3)	-1(2)
Cl(2A)	47(4)	34(5)	55(8)	12(3)	7(5)	1(5)
Cl(2)	47(7)	32(3)	52(2)	-1(4)	-17(4)	13(2)
Cl(3)	69(5)	33(3)	42(4)	6(3)	12(3)	11(3)
C(3AA)	34(7)	85(11)	45(8)	5(7)	1(5)	-1(7)

C(1AA)	51(8)	51(9)	34(7)	16(6)	-1(5)	7(6)
C(0AA)	47(8)	29(7)	96(13)	-9(6)	7(7)	23(8)
N(0AA)	70(8)	41(7)	121(13)	4(6)	51(8)	-7(8)
C(5)	34(6)	42(7)	34(7)	9(5)	1(5)	4(5)
C(6)	44(7)	52(8)	53(8)	-11(6)	21(6)	-2(6)
N(1)	41(5)	26(5)	28(5)	8(4)	8(4)	-10(4)
N(2AA)	78(8)	34(6)	20(5)	-10(5)	2(5)	0(4)
C(3)	63(8)	21(6)	50(8)	-13(6)	-1(6)	-7(6)
C(5AA)	57(12)	51(11)	43(10)	3(11)	-11(11)	20(8)
C(4AA)	154(19)	64(12)	40(10)	52(13)	-27(11)	7(8)
C(6AA)	123(12)	25(5)	45(6)	10(6)	4(7)	9(4)
C(7)	123(12)	25(5)	45(6)	10(6)	4(7)	9(4)
C(8)	123(12)	25(5)	45(6)	10(6)	4(7)	9(4)
C(9)	57(12)	51(11)	43(10)	3(11)	-11(11)	20(8)
C(10)	45(8)	28(8)	8(6)	-5(6)	-4(6)	1(5)
C(2A)	38(14)	21(9)	28(8)	3(10)	3(11)	8(7)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S4. Bond lengths [Å] for $(C_9H_{15}N_3)ZnCl_4$ at 150.0 K with estimated standard deviations in parentheses.

Label	Distances		
Zn(02)-Cl(0A)	2.264(3)	Zn(06)-Cl(0U)	2.217(11)
Zn(02)-Cl(0D)	2.297(4)	Zn(06)-Cl(1A)	2.086(18)
Zn(02)-Cl(0J)	2.218(4)	Zn(06)-Cl(3)	2.271(13)
Zn(02)-Cl(0Q)	2.301(16)	Cl(07)-Zn(8)	2.306(4)
Zn(02)-Cl(2A)	2.27(2)	Cl(08)-Zn(8)	2.287(3)
Zn(03)-Cl(0C)	2.294(4)	Cl(09)-Zn(8)	2.242(4)
Zn(03)-Cl(0K)	2.217(5)	Cl(0B)-Zn(8)	2.279(4)
Zn(03)-Cl(0L)	2.295(4)	Cl(0E)-Zn(0A)	2.297(13)
Zn(03)-Cl(0R)	2.303(4)	Cl(0F)-Zn(2)	2.260(16)
Zn(04)-Cl(0F)	2.237(10)	Cl(0G)-Zn(2)	2.522(12)
Zn(04)-Cl(0G)	2.237(8)	Cl(0H)-Zn(0A)	2.069(12)
Zn(04)-Cl(0I)	2.403(9)	Cl(0I)-Zn(2)	2.034(14)
Zn(04)-Cl(0O)	2.329(10)	Cl(0M)-Zn(0A)	2.276(12)
Zn(04)-Cl(1)	2.205(13)	Cl(0N)-Zn(1)	1.969(11)
Zn(04)-Cl(2)	2.27(2)	Cl(0O)-Cl(1)	0.69(5)
Zn(05)-Cl(0E)	2.176(17)	Cl(0O)-Zn(2)	2.527(16)

Zn(05)-Cl(0H)	2.459(11)	Cl(0P)-Zn(0A)	2.394(13)
Zn(05)-Cl(0M)	2.250(15)	Cl(0S)-Zn(1)	2.405(17)
Zn(05)-Cl(0P)	2.157(16)	Cl(0S)-Cl(1A)	0.636(13)
Zn(06)-Cl(0N)	2.407(11)	Cl(0T)-Zn(1)	2.25(2)
Zn(06)-Cl(0S)	2.213(13)	Cl(0T)-Cl(3)	0.646(12)
Zn(06)-Cl(0T)	2.140(17)	Cl(0U)-Zn(1)	2.328(13)

Table S5. Bond angles [°] for $(C_9H_{15}N_3)ZnCl_4$ at 150.0 K with estimated standard deviations in parentheses.

Label	Angles	Label	Angles
Cl(0A)-Zn(02)-Cl(0D)	108.97(14)	Cl(1)-Cl(0O)-Zn(2)	63.3(14)
Cl(0A)-Zn(02)-Cl(0Q)	110.3(5)	Zn(05)-Cl(0P)-Zn(0A)	8.4(5)
Cl(0A)-Zn(02)-Cl(2A)	106.2(6)	Zn(06)-Cl(0S)-Zn(1)	9.8(4)
Cl(0D)-Zn(02)-Cl(0Q)	99.6(4)	Cl(1A)-Cl(0S)-Zn(06)	70.2(16)
Cl(0J)-Zn(02)-Cl(0A)	114.40(16)	Cl(1A)-Cl(0S)-Zn(1)	64.2(16)
Cl(0J)-Zn(02)-Cl(0D)	110.81(17)	Zn(06)-Cl(0T)-Zn(1)	11.1(4)
Cl(0J)-Zn(02)-Cl(0Q)	111.7(5)	Cl(3)-Cl(0T)-Zn(06)	93.3(16)
Cl(0J)-Zn(02)-Cl(2A)	104.4(5)	Cl(3)-Cl(0T)-Zn(1)	100.9(17)
Cl(2A)-Zn(02)-Cl(0D)	111.9(4)	Zn(06)-Cl(0U)-Zn(1)	10.7(4)
Cl(2A)-Zn(02)-Cl(0Q)	12.4(4)	Zn(04)-Cl(1)-Zn(2)	10.4(2)
Cl(0C)-Zn(03)-Cl(0L)	108.88(16)	Cl(0O)-Cl(1)-Zn(04)	92(2)
Cl(0C)-Zn(03)-Cl(0R)	107.78(16)	Cl(0O)-Cl(1)-Zn(2)	101(2)
Cl(0K)-Zn(03)-Cl(0C)	112.61(16)	Cl(08)-Zn(8)-Cl(07)	108.80(14)
Cl(0K)-Zn(03)-Cl(0L)	110.47(16)	Cl(09)-Zn(8)-Cl(07)	109.79(15)
Cl(0K)-Zn(03)-Cl(0R)	113.10(18)	Cl(09)-Zn(8)-Cl(08)	112.30(14)
Cl(0L)-Zn(03)-Cl(0R)	103.54(17)	Cl(09)-Zn(8)-Cl(0B)	113.59(17)
Cl(0F)-Zn(04)-Cl(0G)	112.9(4)	Cl(0B)-Zn(8)-Cl(07)	106.53(16)
Cl(0F)-Zn(04)-Cl(0I)	112.6(6)	Cl(0B)-Zn(8)-Cl(08)	105.53(14)
Cl(0F)-Zn(04)-Cl(0O)	111.1(5)	Cl(0F)-Zn(2)-Cl(0G)	102.3(5)
Cl(0F)-Zn(04)-Cl(2)	12.2(5)	Cl(0F)-Zn(2)-Cl(0O)	103.5(7)
Cl(0G)-Zn(04)-Cl(0I)	108.1(2)	Cl(0F)-Zn(2)-Cl(1)	101.1(8)
Cl(0G)-Zn(04)-Cl(0O)	102.1(5)	Cl(0G)-Zn(2)-Cl(0O)	89.4(5)
Cl(0G)-Zn(04)-Cl(2)	114.0(7)	Cl(0I)-Zn(2)-Cl(0F)	128.0(7)
Cl(0O)-Zn(04)-Cl(0I)	109.6(4)	Cl(0I)-Zn(2)-Cl(0G)	110.6(5)
Cl(1)-Zn(04)-Cl(0F)	104.9(10)	Cl(0I)-Zn(2)-Cl(0O)	115.6(6)
Cl(1)-Zn(04)-Cl(0G)	118.8(18)	Cl(0I)-Zn(2)-Cl(1)	107.7(10)
Cl(1)-Zn(04)-Cl(0I)	98.9(11)	Cl(0I)-Zn(2)-Cl(2)	116.5(9)
Cl(1)-Zn(04)-Cl(0O)	17.1(13)	Cl(1)-Zn(2)-Cl(0G)	104.8(17)

Cl(1)-Zn(04)-Cl(2)	112.8(13)	Cl(1)-Zn(2)-Cl(0O)	15.4(13)
Cl(2)-Zn(04)-Cl(0I)	101.4(7)	Cl(2)-Zn(2)-Cl(0F)	12.3(5)
Cl(2)-Zn(04)-Cl(0O)	121.3(8)	Cl(2)-Zn(2)-Cl(0G)	105.6(8)
Cl(0E)-Zn(05)-Cl(0H)	108.1(6)	Cl(2)-Zn(2)-Cl(0O)	115.1(9)
Cl(0E)-Zn(05)-Cl(0M)	114.7(7)	Cl(2)-Zn(2)-Cl(1)	111.0(12)
Cl(0M)-Zn(05)-Cl(0H)	99.2(5)	Cl(0N)-Zn(1)-Cl(0S)	121.8(7)
Cl(0P)-Zn(05)-Cl(0E)	115.2(6)	Cl(0N)-Zn(1)-Cl(0T)	108.6(8)
Cl(0P)-Zn(05)-Cl(0H)	105.5(6)	Cl(0N)-Zn(1)-Cl(0U)	109.8(6)
Cl(0P)-Zn(05)-Cl(0M)	112.3(7)	Cl(0N)-Zn(1)-Cl(1A)	112.3(7)
Cl(0S)-Zn(06)-Cl(0N)	111.8(5)	Cl(0N)-Zn(1)-Cl(3)	118.1(7)
Cl(0S)-Zn(06)-Cl(0U)	122.3(6)	Cl(0S)-Zn(1)-Cl(3)	97.3(5)
Cl(0S)-Zn(06)-Cl(3)	108.8(5)	Cl(0T)-Zn(1)-Cl(0S)	94.1(6)
Cl(0T)-Zn(06)-Cl(0N)	97.7(6)	Cl(0T)-Zn(1)-Cl(0U)	111.3(7)
Cl(0T)-Zn(06)-Cl(0S)	102.9(6)	Cl(0T)-Zn(1)-Cl(3)	15.0(3)
Cl(0T)-Zn(06)-Cl(0U)	120.2(7)	Cl(0U)-Zn(1)-Cl(0S)	110.2(6)
Cl(0T)-Zn(06)-Cl(3)	16.5(3)	Cl(0U)-Zn(1)-Cl(3)	96.5(5)
Cl(0U)-Zn(06)-Cl(0N)	99.1(4)	Cl(1A)-Zn(1)-Cl(0S)	15.1(4)
Cl(0U)-Zn(06)-Cl(3)	105.3(5)	Cl(1A)-Zn(1)-Cl(0T)	108.9(8)
Cl(1A)-Zn(06)-Cl(0N)	100.8(6)	Cl(1A)-Zn(1)-Cl(0U)	106.0(7)
Cl(1A)-Zn(06)-Cl(0S)	16.7(4)	Cl(1A)-Zn(1)-Cl(3)	112.3(7)
Cl(1A)-Zn(06)-Cl(0T)	117.9(7)	Cl(0E)-Zn(0A)-Cl(0P)	102.5(5)
Cl(1A)-Zn(06)-Cl(0U)	114.5(7)	Cl(0H)-Zn(0A)-Cl(0E)	118.5(6)
Cl(1A)-Zn(06)-Cl(3)	125.3(7)	Cl(0H)-Zn(0A)-Cl(0M)	111.3(5)
Cl(3)-Zn(06)-Cl(0N)	108.6(5)	Cl(0H)-Zn(0A)-Cl(0P)	110.8(5)
Zn(05)-Cl(0E)-Zn(0A)	10.0(4)	Cl(0M)-Zn(0A)-Cl(0E)	109.2(5)
Zn(04)-Cl(0F)-Zn(2)	10.7(2)	Cl(0M)-Zn(0A)-Cl(0P)	103.2(5)
Zn(04)-Cl(0G)-Zn(2)	7.5(3)	Zn(06)-Cl(1A)-Zn(1)	11.3(3)
Zn(0A)-Cl(0H)-Zn(05)	3.2(7)	Cl(0S)-Cl(1A)-Zn(06)	93.1(17)
Zn(2)-Cl(0I)-Zn(04)	5.2(4)	Cl(0S)-Cl(1A)-Zn(1)	100.8(17)
Zn(05)-Cl(0M)-Zn(0A)	10.3(3)	Zn(2)-Cl(2)-Zn(04)	10.7(2)
Zn(1)-Cl(0N)-Zn(06)	0.2(8)	Zn(06)-Cl(3)-Zn(1)	9.7(4)
Zn(04)-Cl(0O)-Zn(2)	8.8(2)	Cl(0T)-Cl(3)-Zn(06)	70.2(15)
Cl(1)-Cl(0O)-Zn(04)	71.2(14)	Cl(0T)-Cl(3)-Zn(1)	64.1(15)

Table S6. The manganese content for the metal components in the raw material and

that obtained from EDS experiment.

Raw Material (Mn%)		1	5	10	20	30	40	50
Experiment (Mn%)	first	4.7	9.2	3.1	3.6	0.21	7	11.3
	second	0	1.2	0	11	14.6	4.1	6.1
	third	0.39	0	0	4.9	0	8.1	14.4
	average	1.69	3.47	1.03	6.5	4.94	6.4	10.6

Table S7. CIE coordinates of $(C_9H_{15}N_3)ZnCl_4$:Mn^{2+} with different Mn^{2+} feed ratio (0～50%).

Mn^{2+} (%)	0	1	5	10	20	30	40	50
CIE	(0.1627,0.0972)	(0.1736,0.1986)	(0.1924,0.3686)	(0.1979,0.4098)	(0.2067,0.4844)	(0.2119,0.526)	(0.2156,0.5564)	(0.2187,0.5647)

Table S8. CIE coordinates of $(C_9H_{15}N_3)ZnCl_4$:5%Mn^{2+} in the temperature range of 110 to 290 K

Temperature (K)	110 K	140 K	170 K	200 K	230 K	260 K	290 K
CIE	(0.1885, 0.3067)	(0.1897, 0.3157)	(0.1921, 0.3257)	(0.1967, 0.348)	(0.1999, 0.3761)	(0.2028, 0.4052)	(0.2053, 0.4208)

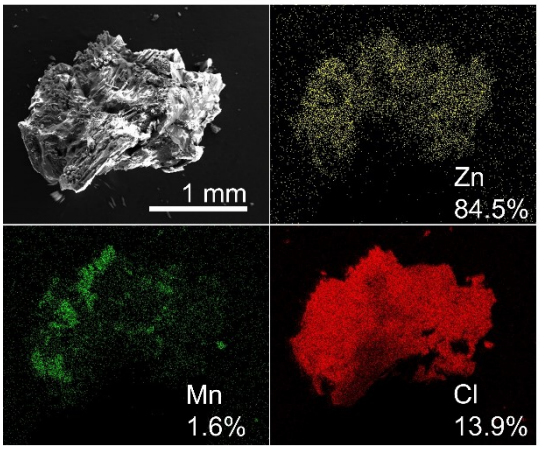

Figure S1. SEM images of $(C_9H_{15}N_3)_2ZnCl_4$: Mn^{2+} (50%) and element mapping images of Zn, Mn, and Cl.

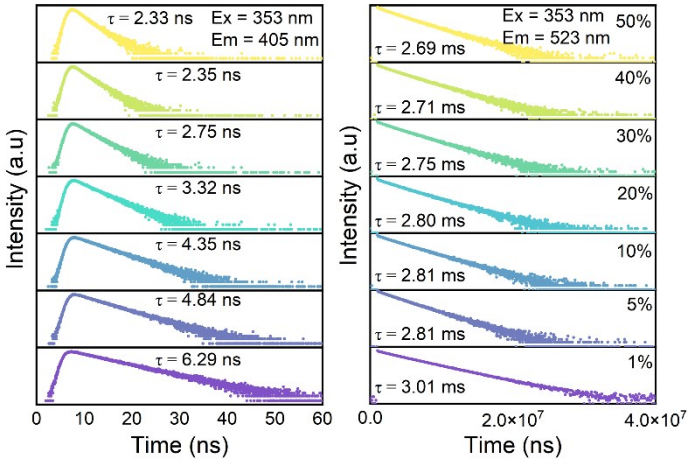

Figure S2. The fluorescence decay lifetime of $(C_9H_{15}N_3)ZnCl_4$: Mn^{2+} with different Mn^{2+} feed ratio (1% ～50%) recorded at 405 and 523 nm at room temperature.

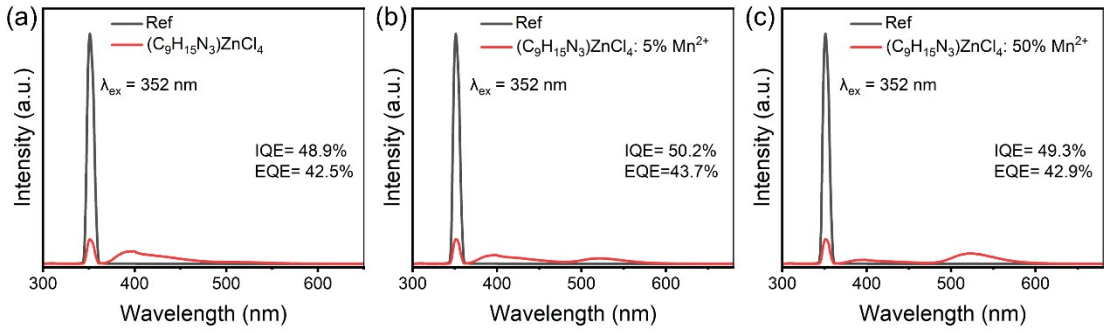

Figure S3. The PL spectra of (a) $(C_9H_{15}N_3)_2ZnCl_4$, (b) $(C_9H_{15}N_3)_2ZnCl_4$: 5%Mn^{2+} and (c) $(C_9H_{15}N_3)_2ZnCl_4$: 50%Mn^{2+} with Al_2O_3 as reference.

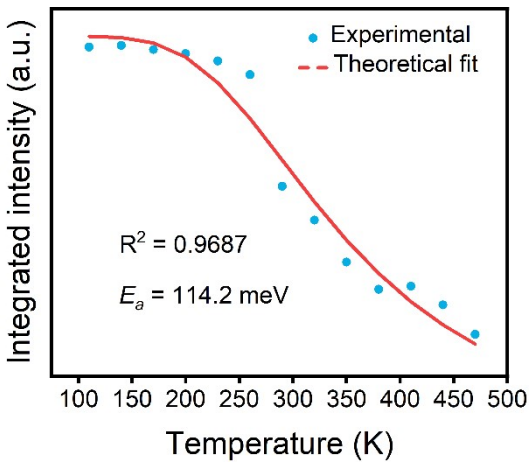

Figure S4. The integrated PL intensity of $(C_9H_{15}N_3)ZnCl_4$ in the range of 110 ~ 470 K as a function of temperature.