Zinc and Cadmium Complexes Based on Bis-(1*H*-tetrazol-5-ylmethyl/ylethyl)-amine Ligands: Structures and Photoluminescence properties

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Table S1. Selected Bond Distances (Å) and Angles (°) for Complexes **1–9**

		complex **1**	
Zn(1)-N(2)	2.163(10)	Zn(1)-N(3)	2.240(9)
Zn(1)-N(5)	2.107(9)	Zn(1)-N(7)	2.079(9)
Zn(1)-O(1W)	2.249(9)	Zn(1)-N(4)	2.099(8)
N(7)-Zn(1)-N(4)	97.7(3)	N(7)-Zn(1)-N(5)	95.9(4)
N(7)-Zn(1)-N(2)	103.5(4)	N(4)-Zn(1)-N(2)	93.8(3)
N(5)-Zn(1)-N(2)	88.0(3)	N(4)-Zn(1)-N(3)	78.2(3)
N(5)-Zn(1)-N(3)	88.3(4)	N(2)-Zn(1)-N(3)	75.7(4)
N(7)-Zn(1)-O(1W)	88.3(4)	N(4)-Zn(1)-O(1W)	87.5(3)
N(5)-Zn(1)-O(1W)	87.8(3)	N(3)-Zn(1)-O(1W)	92.7(4)
		complex **2**	
Zn(1)-N(1)	1.997(3)	Zn(1**d**) -N(2)	2.109(3)
Zn(1**x**) -N(6)	2.003(3)	Zn(1)-N(9)	1.993(3)
Zn(1)-N(5)	2.546(3)		
N(9)-Zn(1)-N(1)	118.02(14)	N(9)-Zn(1)-N(6**c**)	113.86(14)
N(1)-Zn(1)-N(6**c**)	119.78(14)	N(9)-Zn(1)-N(2**d**)	103.94(14)
N(1)-Zn(1)-N(2**d**)	100.21(14)	N(6)[c]-Zn(1)-N(2**d**)	94.92(14)
		complex **3**	
Cd(1)-N(5)	2.328(2)	Cd(1)-N(4)	2.349(2)
Cd(1)-N(3)	2.351(2)	Cd(1)-N(1)	2.447(2)
Cd(1)-N(2)	2.493(2)	Cd(1)-Cl(1)	2.6140(8)
Cd(1)-N(6)	2.807(2)	Cd(2)-Cl(1)	2.6145(8)
Cd(2)-N(7)	2.321(2)	Cd(2)-N(8)	2.311(2)
N(5)-Cd(1)-N(4)	88.87(8)	N(5)-Cd(1)-N(3)	86.79(8)

N(5)-Cd(1)-N(1)	78.62(8)	N(4)-Cd(1)-N(1)	84.40(8)
N(3)-Cd(1)-N(1)	113.40(8)	N(3)-Cd(1)-N(2)	69.07(8)
N(1)-Cd(1)-N(2)	66.83(7)	N(4)-Cd(1)-Cl(1)	85.92(6)
N(3)-Cd(1)-Cl(1)	88.77(6)	N(2)-Cd(1)-Cl(1)	80.92(6)
N(8)-Cd(2)-N(7)	90.86(8)	N(8)-Cd(2)-N(7**h**)	89.14(8)
N(8)-Cd(2)-Cl(1)	94.33(6)	N(7)^{h}-Cd(2)-Cl(1)	86.77(6)
N(7)-Cd(2)-Cl(1)	93.24(6)	N(8)^{h}-Cd(2)-Cl(1**h**)	94.33(6)
N(8)-Cd(2)-Cl(1**h**)	85.67(6)	N(7)^{h}-Cd(2)-Cl(1**h**)	93.24(6)
N(7)-Cd(2)-Cl(1**h**)	86.76(6)		

complex **4**

Cd(1)-N(9)	2.2871(19)	Cd(1)-N(2**i**)	2.288(2)
Cd(1)-O(1)	2.303(2)	Cd(1)-O(2)	2.327(2)
Cd(1)-N(1)	2.3523(19)	Cd(1)-N(5)	2.434(2)
N(9)-Cd(1)-O(1)	88.85(7)	N(2**i**)-Cd(1)-O(1)	86.20(7)
N(9)-Cd(1)-O(2)	85.91(7)	N(2**i**)-Cd(1)-O(2)	93.34(8)
N(2**i**)-Cd(1)-N(1)	94.58(7)	O(1)-Cd(1)-N(1)	99.65(7)
O(2)-Cd(1)-N(1)	86.85(7)	N(9)-Cd(1)-N(5)	72.65(8)
O(1)-Cd(1)-N(5)	91.88(8)	O(2)-Cd(1)-N(5)	90.21(9)
N(1)-Cd(1)-N(5)	71.06(7)		

complex **5**

Cd(1)-N(1)	2.296(2)	Cd(2)-N(6)	2.413(2)
Cd(1)-N(2**k**)	2.324(2)	Cd(1)-N(9**m**)	2.460(2)
Cd(2)-N(8**p**)	2.404(2)	Cd(2)-N(4)	2.307(2)
N(1**j**)-Cd(1)-N(2**k**)	94.85(8)	N(1)-Cd(1)-N(2**k**)	89.03(7)
N(2**k**)-Cd(1)-N(2**l**)	90.75(12)	N(1)-Cd(1)-N(9**m**)	72.31(7)
N(1**j**)-Cd(1)-N(9**m**)	104.04(8)	N(2**l**)-Cd(1)-N(9**m**)	87.08(8)
N(9**m**)-Cd(1)-N(9**n**)	100.93(11)	N(4)-Cd(2)-N(8**p**)	84.90(7)
N(4)-Cd(2)-N(8**q**)	95.10(7)	N(4)-Cd(2)-N(6**o**)	96.99(8)
N(4**o**)-Cd(2)-N(6**o**)	83.01(8)	N(8**p**)-Cd(2)-N(6**o**)	84.05(8)
N(8**p**)-Cd(2)-N(6)	95.95(8)		

complex **6**

Zn(1)-N(1)	2.0287(18)	Zn(1)-N(2**r**)	2.1914(19)
Zn(1)-N(5)	2.184(2)	Zn(1)-N(6)	2.0372(18)
Zn(1)-N(7)	2.0572(18)		
N(1)-Zn(1)-N(6)	110.92(8)	N(1)-Zn(1)-N(7)	116.86(7)
N(1)-Zn(1)-N(5)	89.95(8)	N(6)-Zn(1)-N(5)	86.44(8)
N(7)-Zn(1)-N(5)	87.16(8)	N(1)-Zn(1)-N(2**r**)	96.88(7)
N(6)-Zn(1)-N(2**r**)	92.03(7)	N(7)-Zn(1)-N(2**r**)	88.85(7)

complex **7**

Zn(1)-N(5)	2.122(2)	Zn(1)-N(1)	2.295(2)
Zn(2)-N(3)	2.015(2)	Zn(2)-Cl(1)	2.1819(12)
Zn(2)-N(4)	2.070(3)	Zn(1)-N(6)	2.086(3)
Zn(1)-N(6**t**)	2.124(3)		
N(6)-Zn(1)-N(5)	103.34(8)	N(5**s**)-Zn(1)-N(5)	91.12(12)
N(5)-Zn(1)-N(6**t**)	86.42(8)	N(6)-Zn(1)-N(1)	81.24(8)
N(5)-Zn(1)-N(1)	89.65(8)	N(6**t**)-Zn(1)-N(1)	88.73(7)
N(1)-Zn(1)-N(1**s**)	89.17(11)	N(3)-Zn(2)-N(3**y**)	115.17(14)
N(3)-Zn(2)-N(4)	95.00(7)	N(3)-Zn(2)-Cl(1)	116.55(7)
N(4)-Zn(2)-Cl(1)	114.16(10)		

complex **8**

Cd(1)-N(1)	2.242(2)	Cd(1)-N(9)	2.258(2)
Cd(1)-O(1)	2.316(3)	Cd(1)-N(5)	2.374(2)
Cd(1)-O(3)	2.459(2)	Cd(1)-O(2)	2.472(2)
N(1)-Cd(1)-O(1)	93.91(10)	N(5)-Cd(1)-O(2)	77.97(7)
N(9)-Cd(1)-O(1)	93.56(10)	N(1)-Cd(1)-N(5)	87.60(8)
N(9)-Cd(1)-N(5)	87.33(8)	N(1)-Cd(1)-O(3)	84.67(9)
N(9)-Cd(1)-O(3)	85.77(9)	O(1)-Cd(1)-O(3)	105.39(10)
N(5)-Cd(1)-O(3)	90.33(8)	N(1)-Cd(1)-O(2)	94.61(8)
N(9)-Cd(1)-O(2)	93.71(8)	O(1)-Cd(1)-O(2)	86.31(9)

complex **9**

Cd(1)-O(1**u**)	2.2465(13)	Cd(1)-N(4**v**)	2.3196(16)
Cd(1)-O(1)	2.3284(13)	Cd(1)-N(7**w**)	2.3627(16)
Cd(1)-O(4A)	2.403(7)	Cd(1)-N(8)	2.5047(16)
Cd(1)-O(3B)	2.526(15)	Cd(2)-O(1)	2.2640(12)
Cd(2)-N(1)	2.2859(16)	Cd(2)-N(9)	2.2995(16)
Cd(2)-O(5)	2.3038(15)	Cd(2)-N(5)	2.3994(16)
Cd(2)-N(3**v**)	2.4226(16)	Cd(1**w**) -N(7)	2.3627(16)
Cd(1**u**)-O(1)	2.2465(13)		
O(1**u**)-Cd(1)-O(1)	80.71(5)	N(4**v**)-Cd(1)-O(1)	86.34(5)
O(1**u**)-Cd(1)-N(7**w**)	88.67(5)	N(4**v**)-Cd(1)-N(7**w**)	105.33(6)
O(1**u**)-Cd(1)-O(4A)	79.1(2)	N(4**v**)-Cd(1)-O(4A)	90.6(2)
O(1)-Cd(1)-O(4A)	75.78(19)	N(7**v**)-Cd(1)-O(4A)	112.3(2)
O(1**u**)-Cd(1)-N(8)	102.67(5)	N(4**v**)-Cd(1)-N(8)	84.36(6)
O(1)-Cd(1)-N(8)	88.99(5)	N(7**w**)-Cd(1)-N(8)	83.44(5)
O(1**u**)-Cd(1)-O(3B)	99.44(18)	N(4**v**)-Cd(1)-O(3B)	78.98(17)
O(1)-Cd(1)-O(3B)	113.68(19)	N(7**w**)-Cd(1)-O(3B)	77.92(18)

O(4A)-Cd(1)-O(3B)	40.7(2)	O(1)-Cd(2)-N(1)	97.68(5)
O(1)-Cd(2)-N(9)	89.82(5)	O(1)-Cd(2)-O(5)	94.03(5)
N(1)-Cd(2)-O(5)	98.94(6)	N(9)-Cd(2)-O(5)	93.21(6)
N(1)-Cd(2)-N(5)	86.06(6)	N(9)-Cd(2)-N(5)	86.02(6)
O(5)-Cd(2)-N(5)	87.66(6)	O(1)-Cd(2)-N(3**v**)	82.46(5)
N(1)-Cd(2)-N(3**v**)	85.10(6)	N(9)-Cd(2)-N(3**v**)	83.26(6)
N(5)-Cd(2)-N(3**v**)	95.59(6)		

Symmetry code for **2**: **d:** -x,-y+1,-z+1; **x:** x+1/2,-y+3/2,z+1/2; **c:** x-1/2,-y+3/2,z-1/2. for **3**: **h:** -x+5/3,-y+4/3,-z+1/3. for **4**: **i:** -x,-y+1,-z. for **5**: **m:** x,-y+2,z+1/2; **j:** -x+1,y,-z+1/2; **k:** -x+1,-y+1,-z; **l:** x,-y+1,z+1/2; **n:** -x+1,-y+2,-z; **o:** -x+3/2,-y+3/2,-z; **p:** -x+3/2,y-1/2,-z+1/2; **q:** x,-y+2,z-1/2. for **6**: **r:** -x+2,-y+2,-z+1. for **7**: **t:** x+1/2,y,-z+3/2; **s:** x,-y+5/2,z. for **9**: **u:** -x+2,-y,-z; **v**: -x+2,y+1/2,-z+1/2; **w**: -x+2,-y+1,-z.

Table S2 Hydrogen-bonding geometry (Å, °) for **4** and **8**

D–H···A	D–H	H···A	D···A	D–H···A
Complex **4**				
O(1)-H(1W)···O(3)	0.816(18)	1.905(19)	2.720(3)	175(4)
O(1)-H(2W)···N(6)	0.832(18)	1.948(19)	2.772(3)	170(4)
O(2)-H(3W)···O(3)	0.823(19)	1.923(19)	2.746(3)	178(4)
O(2)-H(4W)···N(3)	0.839(18)	2.04(2)	2.871(3)	170(4)
O(3)-H(5W)···N(4)	0.834(18)	1.96(2)	2.782(3)	171(4)
O(3)-H(6W)···N(8)	0.849(18)	1.964(19)	2.810(3)	175(4)
Complex **8**				
O(2)-H(3W)···N(6)	0.843(19)	1.96(2)	2.777(4)	162(5)
O(2)-H(4W)···N(4)	0.831(19)	1.98(2)	2.805(3)	169(5)
O(3)-H(5W)···N(3)	0.838(19	2.17(2)	2.997(4)	170(5)
O(3)-H(6W)···N(7)	0.85(2)	2.13(2)	2.984(4)	172(5)

Table S3. Emission decay data fitted for $H_3\mathbf{L^1}$, $H_3\mathbf{L^2}$, **1–9**

	τ_1/ns	τ_2/ns	τ_3/ns	A_1%	A_2%	A_3%
$H_3\mathbf{L^1}$	2.63	6.81	0.28	3.13	0.79	35.70
$H_3\mathbf{L^2}$	0.64	2.85	7.54	14.49	3.85	0.71
1	3.02	0.75	8.52	4.56	12.33	0.48
2	3.95	1.16	10.33	4.36	9.14	4.31
3	0.66	3.50	9.89	14.84	3.86	0.50
4	2.53	7.34	0.45	3.90	0.91	19.69

5	0.50	2.77	8.19	17.72	4.26	0.72
6	2.61	0.38	7.57	4.18	23.01	0.93
7	2.47	0.52	6.84	5.87	14.17	0.61
8	0.30	2.44	7.61	35.12	3.21	0.60
9	2.07	0.26	6.83	3.06	41.74	0.57