

Construction of Luminescent Three-Dimensional Ln(III)-Zn(II) Heterometallic Coordination Polymers based on 2-Pyridyl Imidazole Dicarboxylate

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Supporting information

Table S1 Selected bond lengths [Å] and angles [°] for the compounds.^a

Complex 1			
Sm(1)-O(2)	2.362(6)	Zn(1)-O(1)	2.034(7)
Sm(1)-O(2)#1	2.362(6)	Zn(1)-O(4)#4	2.052(7)
Sm(1)-O(2)#2	2.362(6)	Zn(1)-N(2)#4	2.106(7)
Sm(1)-O(2)#3	2.362(6)	Zn(1)-N(1)	2.126(7)
Sm(1)-O(3)#1	2.433(6)	Zn(2)-N(3)	2.086(9)
Sm(1)-O(3)	2.433(6)	Zn(2)-N(3)#5	2.086(9)
Sm(1)-O(3)#2	2.433(6)	Zn(2)-O(1W)	2.153(11)
Sm(1)-O(3)#3	2.433(6)	Zn(2)-O(2W)#5	2.180(8)
Zn(1)-Cl(1)	2.0120(18)	Zn(2)-O(2W)	2.180(8)
O(2)-Sm(1)-O(2)#1	106.9(4)	O(2)-Sm(1)-O(3)#2	79.6(2)
O(2)-Sm(1)-O(2)#2	82.1(4)	O(2)#1-Sm(1)-O(3)#2	138.5(2)
O(2)#1-Sm(1)-O(2)#2	147.9(3)	O(2)#2-Sm(1)-O(3)#2	72.9(2)
O(2)-Sm(1)-O(2)#3	147.9(3)	O(2)#3-Sm(1)-O(3)#2	74.1(3)
O(2)#1-Sm(1)-O(2)#3	82.1(4)	O(3)#1-Sm(1)-O(3)#2	69.7(3)
O(2)#2-Sm(1)-O(2)#3	106.9(4)	O(3)-Sm(1)-O(3)#2	143.3(3)
O(2)-Sm(1)-O(3)#1	74.1(3)	O(2)-Sm(1)-O(3)#3	138.5(2)
O(2)#1-Sm(1)-O(3)#1	72.9(2)	O(2)#1-Sm(1)-O(3)#3	79.6(2)
O(2)#2-Sm(1)-O(3)#1	138.5(2)	O(2)#2-Sm(1)-O(3)#3	74.1(3)
O(2)#3-Sm(1)-O(3)#1	79.6(2)	O(2)#3-Sm(1)-O(3)#3	72.9(2)
O(2)-Sm(1)-O(3)	72.9(2)	O(3)#1-Sm(1)-O(3)#3	143.3(3)
O(2)#1-Sm(1)-O(3)	74.1(3)	O(3)-Sm(1)-O(3)#3	69.7(3)
O(2)#2-Sm(1)-O(3)	79.6(2)	O(3)#2-Sm(1)-O(3)#3	123.1(3)
O(2)#3-Sm(1)-O(3)	138.5(2)	Cl(1)-Zn(1)-O(1)	125.9(4)
O(3)#1-Sm(1)-O(3)	123.1(3)	Cl(1)-Zn(1)-O(4)#4	114.0(4)
O(1)-Zn(1)-O(4)#4	119.8(3)	N(3)-Zn(2)-O(1W)	120.1(3)
Cl(1)-Zn(1)-N(2)#4	101.0(2)	N(3)#5-Zn(2)-O(1W)	120.1(3)
O(1)-Zn(1)-N(2)#4	93.1(3)	N(3)-Zn(2)-O(2W)#5	89.6(4)
O(4)#4-Zn(1)-N(2)#4	80.0(3)	N(3)#5-Zn(2)-O(2W)#5	92.2(4)
Cl(1)-Zn(1)-N(1)	91.8(2)	O(1W)-Zn(2)-O(2W)#5	88.2(3)
O(1)-Zn(1)-N(1)	80.2(3)	N(3)-Zn(2)-O(2W)	92.2(4)
O(4)#4-Zn(1)-N(1)	93.8(3)	N(3)#5-Zn(2)-O(2W)	89.6(4)
N(2)#4-Zn(1)-N(1)	167.1(3)	O(1W)-Zn(2)-O(2W)	88.2(3)
N(3)-Zn(2)-N(3)#5	119.8(5)	O(2W)#5-Zn(2)-O(2W)	176.5(6)
Complex 2			

Eu(1)-O(2)#1	2.361(4)	Zn(1)-O(1)#4	2.029(5)
Eu(1)-O(2)#2	2.361(4)	Zn(1)-O(4)	2.042(5)
Eu(1)-O(2)	2.361(4)	Zn(1)-N(2)	2.122(6)
Eu(1)-O(2)#3	2.361(4)	Zn(1)-N(1)#4	2.133(6)
Eu(1)-O(3)#1	2.440(4)	Zn(2)-N(3)	2.072(6)
Eu(1)-O(3)#3	2.440(4)	Zn(2)-N(3)#5	2.072(6)
Eu(1)-O(3)	2.440(4)	Zn(2)-O(1W)	2.133(9)
Eu(1)-O(3)#2	2.440(4)	Zn(2)-O(2W)#5	2.189(7)
Zn(1)-Cl(1)	1.9818(10)	Zn(2)-O(2W)	2.189(7)
O(2)#1-Eu(1)-O(2)#2	105.8(2)	O(2)#1-Eu(1)-O(3)	138.55(17)
O(2)#1-Eu(1)-O(2)	147.7(2)	O(2)#2-Eu(1)-O(3)	79.44(17)
O(2)#2-Eu(1)-O(2)	83.2(3)	O(2)-Eu(1)-O(3)	73.09(16)
O(2)#1-Eu(1)-O(2)#3	83.2(3)	O(2)#3-Eu(1)-O(3)	74.01(18)
O(2)#2-Eu(1)-O(2)#3	147.7(2)	O(3)#1-Eu(1)-O(3)	69.0(2)
O(2)-Eu(1)-O(2)#3	105.8(2)	O(3)#3-Eu(1)-O(3)	124.0(2)
O(2)#1-Eu(1)-O(3)#1	73.09(16)	O(2)#1-Eu(1)-O(3)#2	74.01(18)
O(2)#2-Eu(1)-O(3)#1	74.01(18)	O(2)#2-Eu(1)-O(3)#2	73.09(16)
O(2)-Eu(1)-O(3)#1	138.55(17)	O(2)-Eu(1)-O(3)#2	79.44(17)
O(2)#3-Eu(1)-O(3)#1	79.44(17)	O(2)#3-Eu(1)-O(3)#2	138.55(17)
O(2)#1-Eu(1)-O(3)#3	79.44(17)	O(3)#1-Eu(1)-O(3)#2	124.0(2)
O(2)#2-Eu(1)-O(3)#3	138.55(17)	O(3)#3-Eu(1)-O(3)#2	69.0(2)
O(2)-Eu(1)-O(3)#3	74.01(18)	O(3)-Eu(1)-O(3)#2	143.0(2)
O(2)#3-Eu(1)-O(3)#3	73.09(16)	Cl(1)-Zn(1)-O(1)#4	124.2(3)
O(3)#1-Eu(1)-O(3)#3	143.0(2)	Cl(1)-Zn(1)-O(4)	117.2(3)
O(1)#4-Zn(1)-O(4)	118.3(2)	N(3)-Zn(2)-O(1W)	121.42(17)
Cl(1)-Zn(1)-N(2)	101.17(16)	N(3)#5-Zn(2)-O(1W)	121.42(17)
O(1)#4-Zn(1)-N(2)	93.1(2)	N(3)-Zn(2)-O(2W)#5	88.3(3)
O(4)-Zn(1)-N(2)	80.10(19)	N(3)#5-Zn(2)-O(2W)#5	92.8(3)
Cl(1)-Zn(1)-N(1)#4	91.83(17)	O(1W)-Zn(2)-O(2W)#5	89.0(2)
O(1)#4-Zn(1)-N(1)#4	79.7(2)	N(3)-Zn(2)-O(2W)	92.8(3)
O(4)-Zn(1)-N(1)#4	93.7(2)	N(3)#5-Zn(2)-O(2W)	88.3(3)
N(2)-Zn(1)-N(1)#4	167.0(2)	O(1W)-Zn(2)-O(2W)	89.0(2)
N(3)-Zn(2)-N(3)#5	117.2(3)	O(2W)#5-Zn(2)-O(2W)	178.0(4)

Complex 3

Tb(1)-O(2)#1	2.335(5)	Zn(1)-O(1)#4	2.040(5)
Tb(1)-O(2)#2	2.335(5)	Zn(1)-O(4)	2.053(5)
Tb(1)-O(2)	2.335(5)	Zn(1)-N(2)	2.115(6)
Tb(1)-O(2)#3	2.335(5)	Zn(1)-N(1)#4	2.134(6)
Tb(1)-O(3)#1	2.425(5)	Zn(2)-N(3)	2.072(6)
Tb(1)-O(3)#3	2.425(5)	Zn(2)-N(3)#5	2.072(6)
Tb(1)-O(3)	2.425(5)	Zn(2)-O(1W)	2.136(8)
Tb(1)-O(3)#2	2.425(5)	Zn(2)-O(2W)#5	2.165(8)
Zn(1)-Cl(1)	1.9669(9)	Zn(2)-O(2W)	2.165(8)
O(2)#1-Tb(1)-O(2)#2	105.8(3)	O(2)#1-Tb(1)-O(3)	138.35(17)

O(2)#1-Tb(1)-O(2)	147.8(2)	O(2)#2-Tb(1)-O(3)	79.55(17)
O(2)#2-Tb(1)-O(2)	83.2(3)	O(2)-Tb(1)-O(3)	73.17(16)
O(2)#1-Tb(1)-O(2)#3	83.2(3)	O(2)#3-Tb(1)-O(3)	73.97(18)
O(2)#2-Tb(1)-O(2)#3	147.8(2)	O(3)#1-Tb(1)-O(3)	68.8(2)
O(2)-Tb(1)-O(2)#3	105.8(3)	O(3)#3-Tb(1)-O(3)	124.1(2)
O(2)#1-Tb(1)-O(3)#1	73.17(16)	O(2)#1-Tb(1)-O(3)#2	73.97(18)
O(2)#2-Tb(1)-O(3)#1	73.97(18)	O(2)#2-Tb(1)-O(3)#2	73.17(16)
O(2)-Tb(1)-O(3)#1	138.35(17)	O(2)-Tb(1)-O(3)#2	79.55(17)
O(2)#3-Tb(1)-O(3)#1	79.55(17)	O(2)#3-Tb(1)-O(3)#2	138.35(17)
O(2)#1-Tb(1)-O(3)#3	79.55(17)	O(3)#1-Tb(1)-O(3)#2	124.1(2)
O(2)#2-Tb(1)-O(3)#3	138.35(17)	O(3)#3-Tb(1)-O(3)#2	68.8(2)
O(2)-Tb(1)-O(3)#3	73.97(18)	O(3)-Tb(1)-O(3)#2	143.3(2)
O(2)#3-Tb(1)-O(3)#3	73.17(16)	Cl(1)-Zn(1)-O(1)#4	122.8(3)
O(3)#1-Tb(1)-O(3)#3	143.3(2)	Cl(1)-Zn(1)-O(4)	118.1(3)
O(1)#4-Zn(1)-O(4)	118.9(2)	N(3)-Zn(2)-O(1W)	121.51(19)
Cl(1)-Zn(1)-N(2)	101.50(16)	N(3)#5-Zn(2)-O(1W)	121.51(19)
O(1)#4-Zn(1)-N(2)	92.8(2)	N(3)-Zn(2)-O(2W)#5	88.0(3)
O(4)-Zn(1)-N(2)	80.0(2)	N(3)#5-Zn(2)-O(2W)#5	92.8(3)
Cl(1)-Zn(1)-N(1)#4	91.48(17)	O(1W)-Zn(2)-O(2W)#5	89.2(2)
O(1)#4-Zn(1)-N(1)#4	79.7(2)	N(3)-Zn(2)-O(2W)	92.8(3)
O(4)-Zn(1)-N(1)#4	94.2(2)	N(3)#5-Zn(2)-O(2W)	88.0(3)
N(2)-Zn(1)-N(1)#4	167.0(2)	O(1W)-Zn(2)-O(2W)	89.2(2)
N(3)-Zn(2)-N(3)#5	117.0(4)	O(2W)#5-Zn(2)-O(2W)	178.3(4)
Complex 4			
Tb(1)-O(3)#1	2.233(3)	Tb(1)-O(2)	2.609(3)
Tb(1)-O(7)#2	2.330(3)	Zn(1)-O(4)#3	2.116(3)
Tb(1)-O(5)	2.331(3)	Zn(1)-N(1)	2.119(3)
Tb(1)-O(2W)	2.364(3)	Zn(1)-N(3)#4	2.125(3)
Tb(1)-O(1W)	2.378(3)	Zn(1)-O(3W)	2.126(3)
Tb(1)-O(2)#1	2.393(3)	Zn(1)-N(2)#3	2.128(3)
Tb(1)-O(1)	2.454(3)	Zn(1)-O(1)	2.283(3)
O(3)#1-Tb(1)-O(7)#2	79.82(12)	O(7)#2-Tb(1)-O(2)	134.77(10)
O(3)#1-Tb(1)-O(5)	85.63(12)	O(5)-Tb(1)-O(2)	73.81(10)
O(7)#2-Tb(1)-O(5)	146.05(11)	O(2W)-Tb(1)-O(2)	118.65(11)
O(3)#1-Tb(1)-O(2W)	88.23(12)	O(1W)-Tb(1)-O(2)	69.72(10)
O(7)#2-Tb(1)-O(2W)	74.81(12)	O(2)#1-Tb(1)-O(2)	64.84(11)
O(5)-Tb(1)-O(2W)	74.23(12)	O(1)-Tb(1)-O(2)	51.19(9)
O(3)#1-Tb(1)-O(1W)	114.39(12)	O(4)#3-Zn(1)-N(1)	90.23(12)
O(7)#2-Tb(1)-O(1W)	72.15(11)	O(4)#3-Zn(1)-N(3)#4	169.73(14)
O(5)-Tb(1)-O(1W)	141.53(11)	N(1)-Zn(1)-N(3)#4	90.96(13)
O(2W)-Tb(1)-O(1W)	135.11(11)	O(4)#3-Zn(1)-O(3W)	92.23(13)
O(3)#1-Tb(1)-O(2)#1	76.55(11)	N(1)-Zn(1)-O(3W)	97.89(13)
O(7)#2-Tb(1)-O(2)#1	125.31(11)	N(3)#4-Zn(1)-O(3W)	97.71(13)
O(5)-Tb(1)-O(2)#1	79.77(11)	O(4)#3-Zn(1)-N(2)#3	77.86(12)

O(2W)-Tb(1)-O(2)#1	150.76(11)	N(1)-Zn(1)-N(2)#3	166.67(13)
O(1W)-Tb(1)-O(2)#1	74.12(10)	N(3)#4-Zn(1)-N(2)#3	99.71(13)
O(3)#1-Tb(1)-O(1)	165.79(11)	O(3W)-Zn(1)-N(2)#3	88.64(13)
O(7)#2-Tb(1)-O(1)	97.50(11)	O(4)#3-Zn(1)-O(1)	86.41(12)
O(5)-Tb(1)-O(1)	89.19(11)	N(1)-Zn(1)-O(1)	75.04(11)
O(2W)-Tb(1)-O(1)	77.62(11)	N(3)#4-Zn(1)-O(1)	84.04(13)
O(1W)-Tb(1)-O(1)	77.49(11)	O(3W)-Zn(1)-O(1)	172.78(11)
O(2)#1-Tb(1)-O(1)	115.53(9)	N(2)#3-Zn(1)-O(1)	97.99(12)
O(3)#1-Tb(1)-O(2)	138.61(10)		

^aSymmetry transformations used to generate equivalent atoms: #1 $-x + 3/4, -y + 3/4, z$, #2 $x, -y + 3/4, -z + 3/4$, #3 $-x + 3/4, y, -z + 3/4$, #4 $x + 1/4, y + 1/4, -z + 1$, #5 $-x + 1/4, -y + 5/4, z$, #6 $x - 1/4, y - 1/4, -z + 1$, #7 $-x - 1/4, -y + 3/4, z$, #8 $-x + 3/2, -y + 1, -z + 3/2$ for complexes **1, 2 and 3**; #1 $-x + 1, -y + 1, -z + 2$, #2 $-x + 1, y - 1/2, -z + 5/2$, #3 $x, -y + 1/2, z + 1/2$, #4 $-x, y + 1/2, -z + 3/2$ for complex **4**.

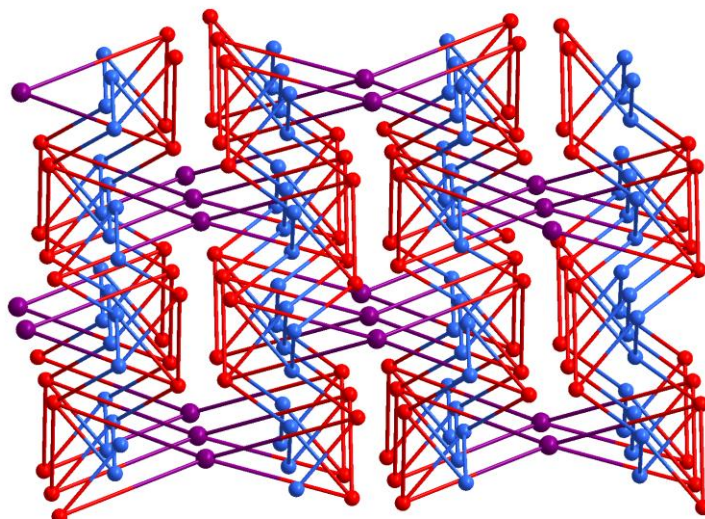


Figure S1. The (3,4)-connected network topology in complexes **1-3**.