

Supporting Information

For

Semidirected vs. holodirected coordination and single component white light luminescence in Pb(II) complexes

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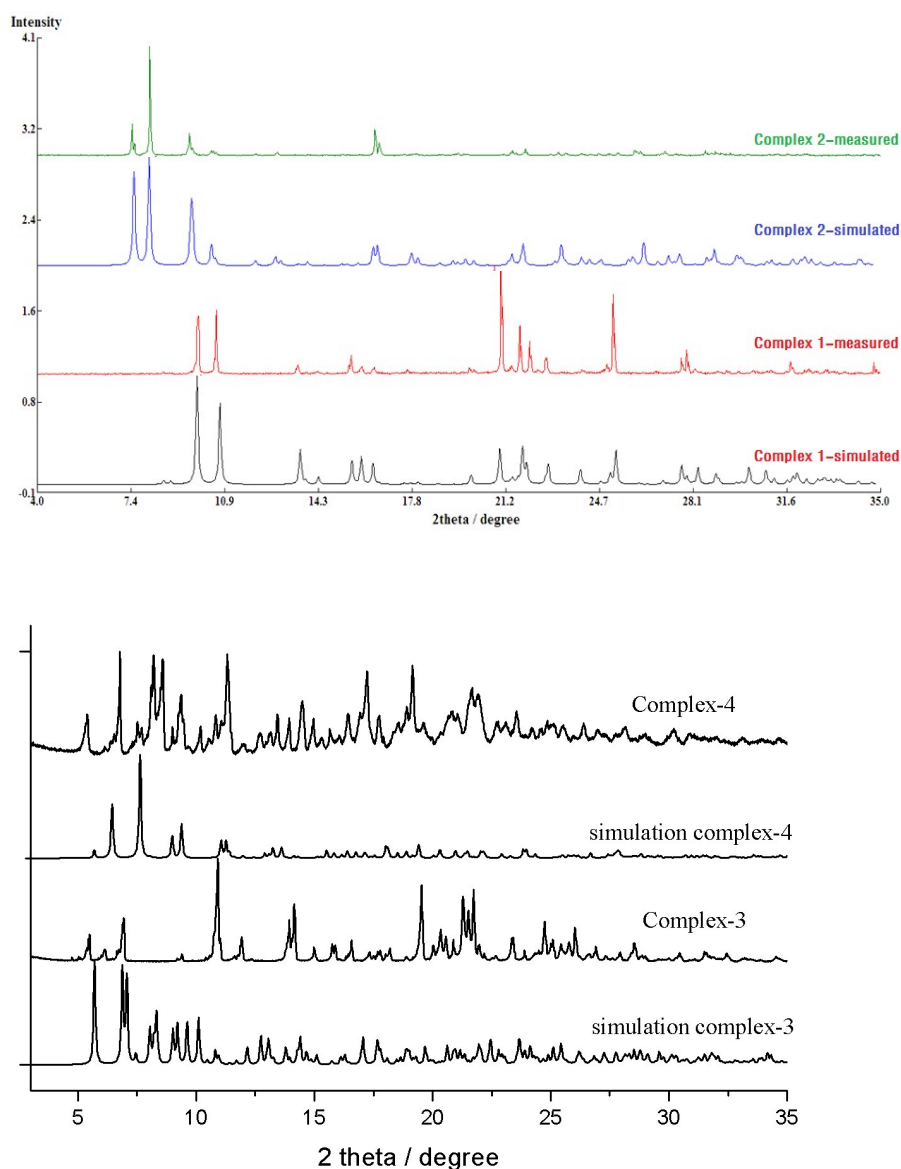
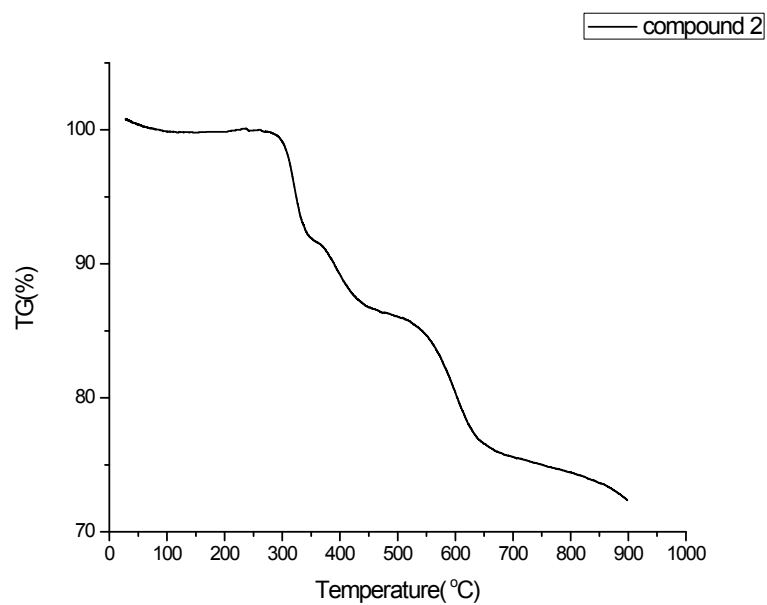
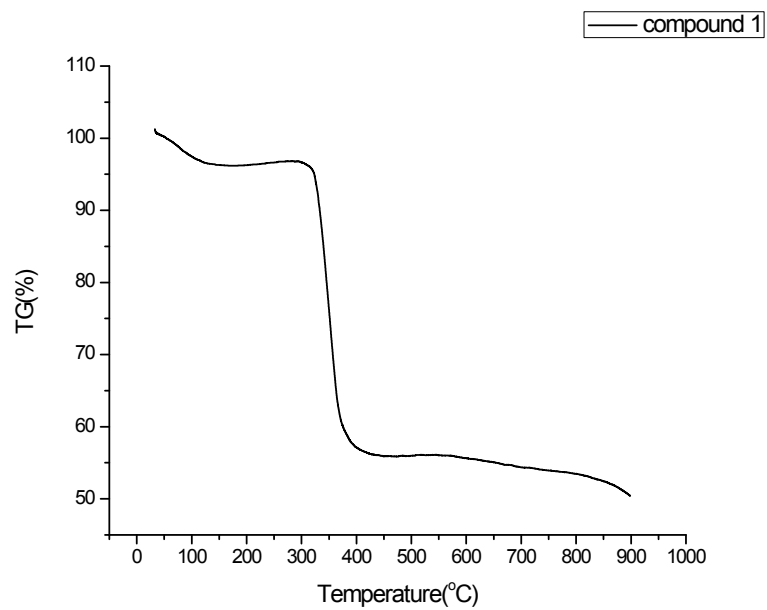


Fig. S1 PXRD patterns of complexes 1 – 4.



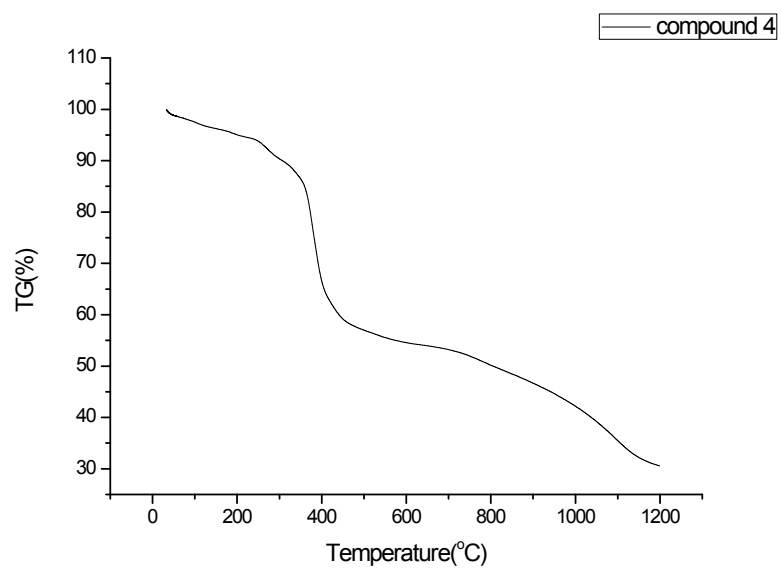
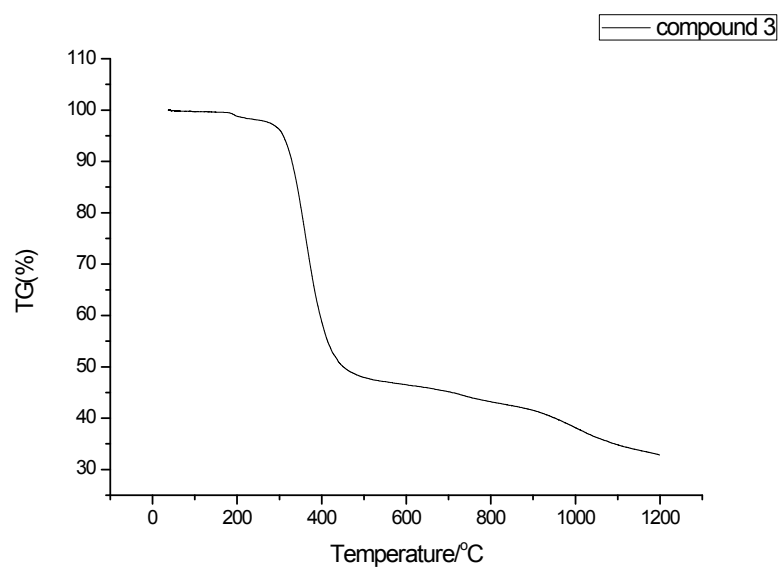
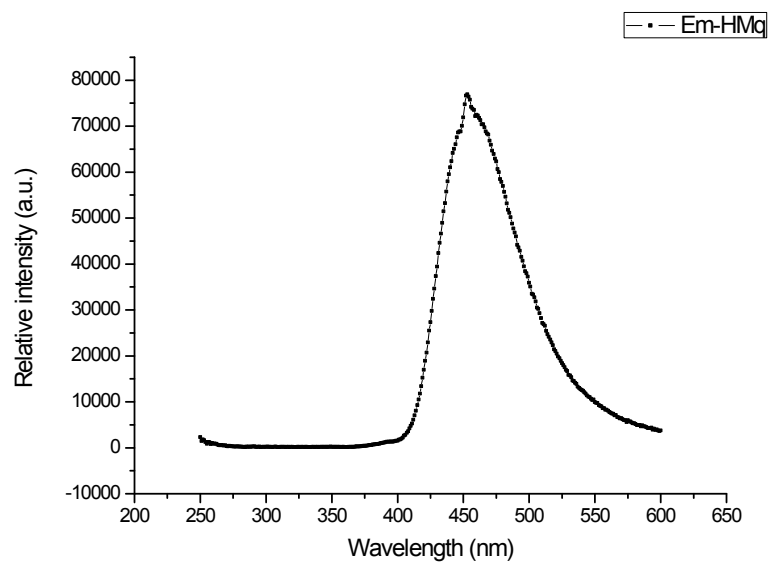
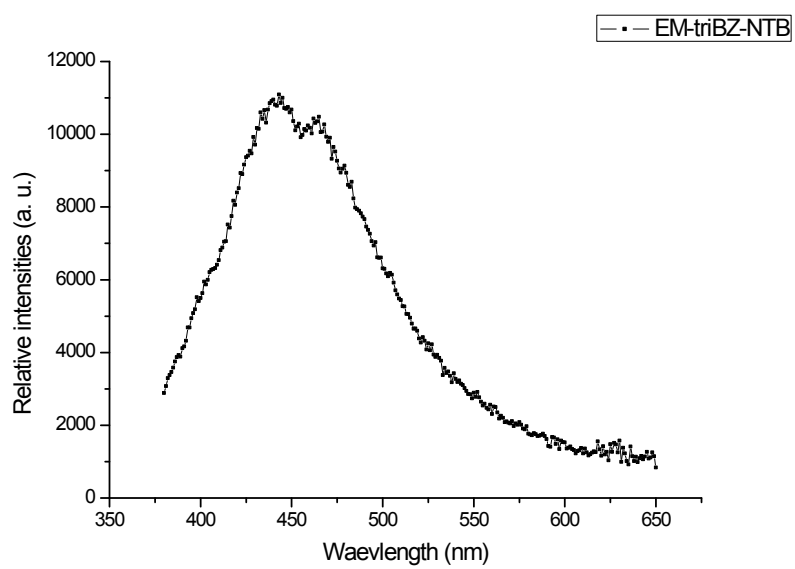


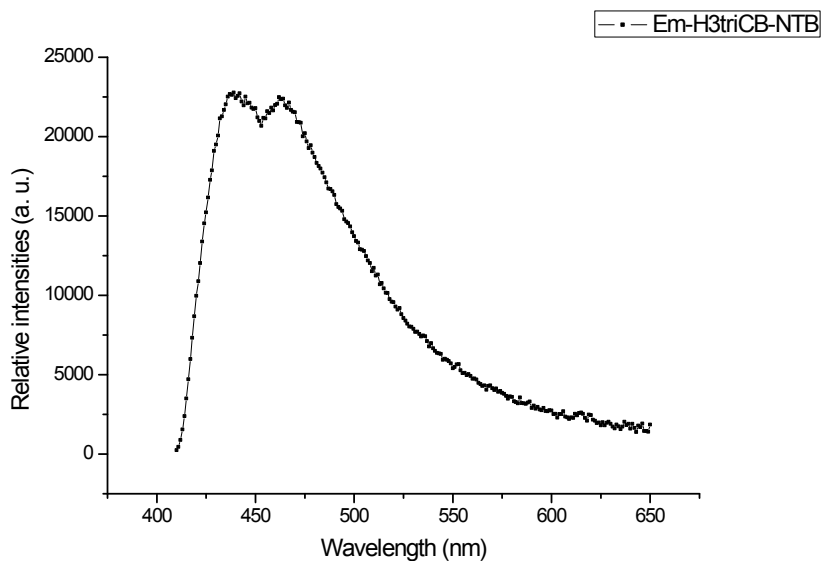
Fig. S2 TG curves of complexes **1** – **4**.



a)



b)



c)

Fig. S3 Emission spectra of the ligands HMq (a), triNB-NTB (b) and H₃triCB-NTB (c).

Table S1 Selected bond lengths and angles for complexes 1-4.

Complex 1

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O4	Pb2	2.277(4)	Pb2	N11	2.534(4)
O8	Pb2	2.281(5)	Pb2	N14	2.537(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Pb2	O8	102.66(17)	N11	Pb2	N14	126.99(12)

Complex 2

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O7	Pb1	2.349(4)	Pb2	O2	2.334(5)
O2	Pb1	2.641(5)	Pb2	O25	2.471(5)
O25	Pb1	2.352(4)	Pb2	O2 ¹	2.560(4)
N1	Pb1	2.485(4)	Pb2	O7	2.512(5)
N2	Pb1 ²	2.728(4)	Pb2	N22	2.565(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O7	Pb1	O2	73.48(17)	O2 ¹	Pb2	O2	67.11(2)
O7	Pb1	O25	70.83(16)	O2 ¹	Pb2	O5	81.74(2)
O2	Pb1	N2	94.41(16)	O2	Pb2	O7	76.22(2)
N1	Pb1	N2	107.09(16)	O2	Pb2	N22	67.35(2)
N1	Pb1	O25	69.22(16)	N7	Pb2	N22	75.63(16)

¹ '-x, -y, -z'

Complex 3

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N16	Pb1	2.671(3)	N9	Pb1	2.658(3)
N13	Pb1	2.658(3)	N6	Pb1	2.706(3)
N19	Pb1	2.652(4)	N3	Pb1	2.737(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N16	Pb1	N6	173.59(10)	N19	Pb1	N13	94.84(10)
N16	Pb1	N3	88.75(10)	N19	Pb1	N9	85.24(10)
N13	Pb1	N16	100.06(10)	N19	Pb1	N6	78.29(11)
N13	Pb1	N6	85.67(10)	N19	Pb1	N3	172.55(10)
N13	Pb1	N3	81.32(10)	N9	Pb1	N16	77.53(10)
N19	Pb1	N16	98.23(10)	N9	Pb1	N13	177.57(9)
N9	Pb1	N3	98.87(10)	N9	Pb1	N6	96.73(10)
N6	Pb1	N3	94.99(10)				

Complex 4

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N6	Zn2	2.044(8)	O6	Pb1 ²	2.533(16)
N2	Zn 2	2.063(10)	O5	Pb1 ²	2.699(14)
N4	Zn 2	2.054(10)	Cl1	Cd2	2.277(3)
N7	Zn 2	2.472(9)	Cl2	Pb1	2.589(4)
O2	Pb1	2.680(17)	Pb1	O2 ¹	2.676(15)
O2	Pb1 ¹	2.677(15)	Pb1	O6 ³	2.533(16)
O1	Pb1	2.431(13)	Pb1	O5 ³	2.699(14)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N6	Zn 2	N2	114.3(3)	O2	Pb1	O2 ¹	76.0(4)
N6	Zn 2	N7	73.2(3)	O2 ¹	Pb1	O5 ³	110.7(4)
N6	Zn 2	Cl1	106.3(3)	O2	Pb1	O5 ³	165.1(6)
N2	Zn 2	N7	74.3(3)	O1	Pb1	O2 ¹	124.4(5)
N4	Zn 2	N6	112.9(4)	O1	Pb1	O2	48.6(4)
N4	Zn 2	N2	110.5(4)	O1	Pb1	O6 ³	75.2(5)
N4	Zn 2	N7	74.0(4)	O1	Pb1	O5 ³	124.2(5)
N4	Zn 2	Cl1	107.1(3)	O1	Pb1	Cl2	95.8(5)
Cl1	Zn 2	N7	178.9(3)	O6 ³	Pb1	O2	120.6(4)
O6 ³	Pb1	Cl2	86.6(5)	O6 ³	Pb1	O2 ¹	156.3(4)
Cl2	Pb1	O2 ¹	78.6(4)	O6 ³	Pb1	O5 ³	49.2(4)
Cl2	Pb1	O2	82.2(4)	Cl2	Pb1	O5 ³	86.0(5)

¹1-X, -1-Y, 1-Z; ²1+X, 1+Y, 1+Z; ³-1+X, -1+Y, -1+Z