Supporting information

X-ray Crystallography

The single-crystal X-ray diffraction data for complexes 1–3 were collected on a Rigaku R-AXIS RAPID IP or a Bruker Smart Apex CCD diffractometer equipped with graphite-monochromated Mo Kα radiation (λ = 0. 71073 Å), operating at 293 ± 2 K. The structures were solved by direct method and refined by full-matrix least squares based on F^2 using the SHELXTL 5.1 software package. The hydrogen atoms residing in the carbon atoms were located geometrically. All non-hydrogen atoms were refined anisotropically. Crystallographic data are given in Table S1. CCDC reference numbers for complexes 1–3 are No. 236562, 32417 and 232419, respectively.

Table S1 Crystal Data and Structure Refinement for **M1**

Data	**Zn1**	**Cd1**	**Hg1**
Formula	$C_{33}H_{43}N_3Cl_2Zn$	$C_{33}H_{43}N_3Cl_2Cd$	$C_{33}H_{43}N_3Cl_2Hg$
Fw	617.97	664.67	752.85
crystal system/ space group	Triclinic		
	P-1		
a / Å	8.808(2)	8.884 (2)	8.847 (2)
b/ Å	9.688(2)	9.967(2)	9.853(2)
c/ Å	21.127(5)	21.213(4)	21.037(4)
α/°	83.056(4)	81.02(3)	80.47(3)
β/°	88.635(4)	88.52(3)	88.41(3)
γ/°	66.246(4)	66.52(3)	66.89(3)
Volume (Å^3)	1637.4(6)	1700.3(6)	1662.0(6)
Z	2	2	2
D_{calcd}, g m^{-3}	1.253	2.805	3.904
F(000)	652	960	1666
θ range for data collection	1.94 ° to 26.10°	2.26° to 27.48°	2.28° to 27.48°
limiting indices	-10 ≤ h ≤10	–11 ≤ h ≤ 11	0 ≤ h ≤ 11
	-11 ≤ k ≤ 11	–27 ≤ l ≤ 27	–11 ≤ k ≤ 12
	-25 ≤ l ≤24	–12 ≤ k ≤ 12	–27 ≤ l ≤ 27
absorption correction	Semi-empirical		
data/restraints/parameters	6289 / 0 / 352	7213/78/352	7359/12/352
goodness-of-fit on F^2	0.972	1.019	1.025
final *R* indices [$I>2\sigma(I)$]	0.0464	0.0736	0.0560
R_1[a]			
R indices (all data)wR_2[b]	0.0935	0.1603	0.1458

[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 Bond lengths [Å] and angles [°] for **Zn1**.

Zn(1)-N(2)	2.098(2)	Zn(1)-Cl(1)	2.2509(9)
Zn(1)-Cl(2)	2.2131(9)	Zn(1)-N(3)	2.297(2)
Zn(1)-N(1)	2.313(2)		
N(2)-Zn(1)-Cl(2)	142.12(6)	N(2)-Zn(1)-N(1)	72.41(8)
N(2)-Zn(1)-Cl(1)	98.40(6)	Cl(2)-Zn(1)-N(1)	98.27(6)
Cl(2)-Zn(1)-Cl(1)	119.47(4)	Cl(1)-Zn(1)-N(1)	102.67(6)
N(2)-Zn(1)-N(3)	72.88(8)	N(3)-Zn(1)-N(1)	139.88(8)
Cl(2)-Zn(1)-N(3)	96.82(6)	C(1)-N(1)-Zn(1)	114.48(18)
Cl(1)-Zn(1)-N(3)	101.71(6)	C(10)-N(1)-Zn(1)	125.30(16)
C(7)-N(3)-Zn(1)	113.86(19)	C(2)-N(2)-Zn(1)	119.08(17)
C(22)-N(3)-Zn(1)	125.36(16)	C(6)-N(2)-Zn(1)	118.08(18)

Table S3 Bond lengths [Å] and angles [°] for **Cd1**.

Cd(1)-N(2)	2.331(5)	Cd(1)-N(3)	2.467(5)
Cd(1)-Cl(1)	2.411(2)	Cd(1)-N(1)	2.480(5)
Cd(1)-Cl(2)	2.451(2)		
N(2)-Cd(1)-Cl(1)	139.19(14)	Cl(1)-Cd(1)-N(3)	99.01(14)
N(2)-Cd(1)-Cl(2)	98.71(14)	Cl(2)-Cd(1)-N(3)	101.71(13)
Cl(1)-Cd(1)-Cl(2)	122.05(9)	N(2)-Cd(1)-N(1)	68.14(16)
N(2)-Cd(1)-N(3)	68.29(17)	Cl(1)-Cd(1)-N(1)	100.81(13)
Cl(2)-Cd(1)-N(1)	103.80(13)	N(3)-Cd(1)-N(1)	131.99(16)

Table S4 Bond lengths [Å] and angles [°] for **Hg1**.

Hg(1)-Cl(1)	2.364(3)	Hg(1)-N(1)	2.513(6)
Hg(1)-N(2)	2.399(6)	Hg(1)-N(3)	2.533(7)
Hg(1)-Cl(2)	2.418(3)		
Cl(1)-Hg(1)-N(2)	134.53(17)	C(1)-N(1)-C(10)	121.4(7)
Cl(1)-Hg(1)-Cl(2)	130.99(11)	C(1)-N(1)-Hg(1)	117.0(6)
N(2)-Hg(1)-Cl(2)	94.42(17)	C(10)-N(1)-Hg(1)	121.6(5)
Cl(1)-Hg(1)-N(1)	98.27(19)	C(2)-N(2)-C(6)	119.6(7)
N(2)-Hg(1)-N(1)	65.8(2)	C(2)-N(2)-Hg(1)	118.9(5)
Cl(2)-Hg(1)-N(1)	101.10(18)	C(6)-N(2)-Hg(1)	119.1(5)
Cl(1)-Hg(1)-N(3)	100.86(19)	C(7)-N(3)-C(22)	120.0(7)
N(2)-Hg(1)-N(3)	65.4(2)	C(7)-N(3)-Hg(1)	118.4(5)
Cl(2)-Hg(1)-N(3)	102.61(18)	C(22)-N(3)-Hg(1)	121.4(5)
N(1)-Hg(1)-N(3)	126.6(2)		

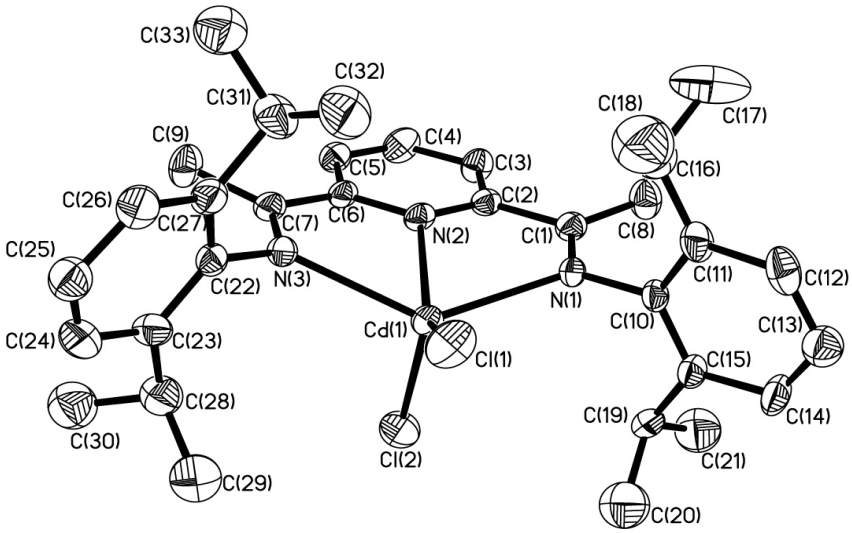

Fig. S1 Molecular structure of complex **Cd1**.

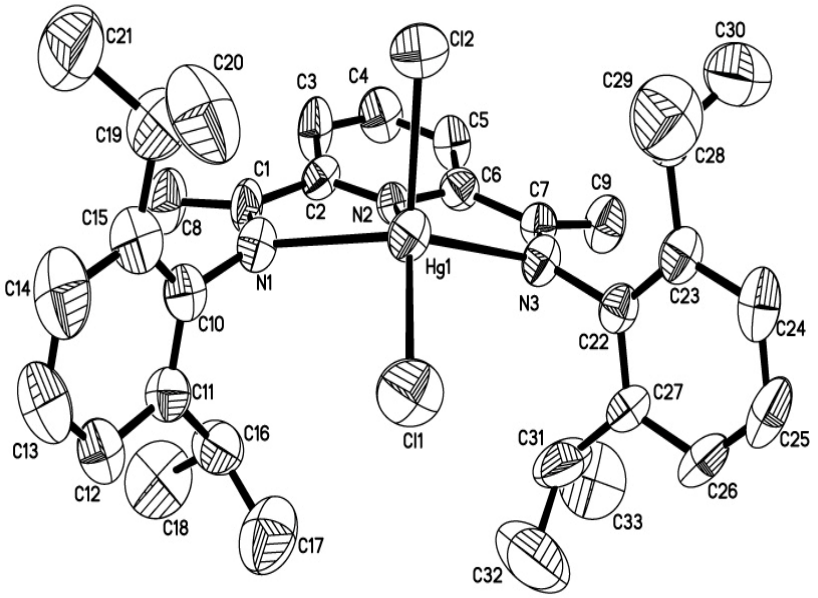

Fig. S2 Molecular structure of complex **Hg1**.

Characterizations of ligand and complexes

Preparation of 2,6-Bis[1-(2,6-diisopropylphenylimino)ethyl]pyridine (L^2): Complex L^2 was prepared as the method described in the part of Experimental Section. Pure L^2 was obtained in 86% yield (6.35 g) upon recrystallization from

methanol. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.60 (d, J = 7.8 Hz, 2 H, Py-H_m), 7.98 (t, J = 7.8 Hz, 1 H, Py-H_p), 7.21–7.13 (m, 6 H, Ar-*H*), 2.78 (sept, J = 6.8 Hz, 4 H, C*H*Me$_2$), 2.30 (s, 6 H, N=C*Me*), 1.19 (dd, J = 6.8 Hz, 24 H, CH*Me*$_2$) ppm. IR (KBr): ν = 3068 (w), 2960 (s), 2925 (w), 2870 (w), 1646 (vs), 1588 (w), 1571 (w), 1455 (m), 1438 (m), 1406 (w), 1383 (w), 1368 (s), 1321 (w), 1301 (w), 1255 (w), 1240 (m), 1195 (m), 1121 (m), 1103 (w), 1079 (w), 1059 (w), 1041 (w), 994 (w), 961 (w), 936 (w), 886 (w), 829 (m), 801 (w), 770 (s), 758 (w), 744 (w), 691 (w), 634 (w), 533 (w), 443 (w) cm^{-1}. $C_{33}H_{43}N_3$ (481.7): calcd. C 82.28, H 9.00, N 8.72; found C 82.50, H 8.91, N 8.65.

Synthesis of 2,6-bis[1-(2,6-diisopropylphenylimino)ethyl]pyridineZnCl$_2$ (2) Complex **Zn1** was prepared as the method described in the part of Experimental Section. Yield: 85%. ^{1}H NMR (500 MHz DMSO-d$_6$, ppm): δ 8.47 (d, 2H, J = 6.5 Hz, Py-H_m), 8.12 (t, 1H, J = 6.5 Hz, Py-H_p), 7.10–6.93 (m, 6H, Ar-*H*), 2.18 (s, 6H, N=C*Me*), 1.98 (s, 12H, C*Me*). IR (KBr, cm^{-1}): 3084w, 3024w, 2960w, 2920w, 2247w, 1636s, 1589s, 1470s, 1440m, 1373s, 1317w, 1260s, 1215s, 1163w, 1148w, 1111w, 1091w, 1024m, 982w, 966w, 920w, 820s, 814s, 783m, 768s, 743m, 697w, 669w, 636w, 584w, 556w, 423w. *Anal.* Calc. for $C_{27}H_{30}N_4Cl_2Zn$: C, 59.30; H, 5.53; N, 10.25%; Found: C, 59.48; H, 5.40; N, 10.56%.

Synthesis of 2,6-bis[1-(2,6-diisopropylphenylimino)ethyl]pyridineCdCl$_2$ (2) Complex **Cd1** was prepared as the method described in the part of Experimental Section. Yield: 177 mg (76%). ^{1}H NMR (300 MHz, CD_3CN): δ = 8.51 (quint, J = 6.9 Hz, 3 H, Py-*H*), 7.27–7.18 (m, 6 H, Ar-*H*), 2.89 (sept, J = 6.6 Hz, 4 H, C*H*Me$_2$), 2.40 (s, 6 H, N=C*Me*), 1.22 (dd, J = 6.6 Hz, 24 H, CH*Me*$_2$) ppm. IR (KBr): ν = 3084 (w), 3063 (w), 2965(s), 2925 (m), 2870 (w), 1636 (s), 1584 (s), br 1457 (m), 1371 (s), 1329 (w), 1306 (w), 1249 (s), 1203 (m), 1106 (m), 1054 (w), 1039 (w), 1017 (w), 979 (w), 937 (w), 819 (m), 796 (m), 775 (m), 758 (w), 744 (w), 716 (w), 697 (w), 637 (w), 529 (w), 468 (w), 445 (w), 432 (w) cm^{-1}. $C_{33}H_{43}N_3CdCl_2$ (664.7): calcd. C 59.60, H 6.52, N 6.32; found: C 59.99, H 6.85, N 6.68.

Synthesis of 2,6-bis[1-(2,6-diisopropylphenylimino)ethyl]pyridineHgCl$_2$ (2)

Complex **Hg1** was prepared as the method described in the part of Experimental Section. Yield 78%. ^{1}H NMR (300 MHz, CD_3CN): δ = 8.52 (s, 3 H, Py-*H*), 7.26–7.18 (m, 6 H, Ar-*H*), 2.87 (sept, *J* = 6.8 Hz, 4 H, C*H*Me$_2$), 2.39 (s, 6 H, N=C*Me*), 1.23 (dd, *J* = 6.8 Hz, 24 H, CH*Me*$_2$) ppm. IR (KBr, cm^{-1}): 3088 (w), 3059 (w), 2960 (s), 2925 (m), 2865 (m), 1638 (s), 1581 (s), br 1455 (s), 1366 (s), 1329 (m), 1301 (m), 1244 (s), 1202 (s), 1105 (m), 1056 (m), 978 (w), 936 (m), 819 (m), 793 (s), 774 (s), 759 (w), 715 (w), 634 (w), 554 (w). Calc. for $C_{33}H_{43}N_3HgCl_2$: C, 52.62; H, 5.75; N, 5.58. Found: C, 52.88; H, 5.96; N 5.89.

Luminescent properties

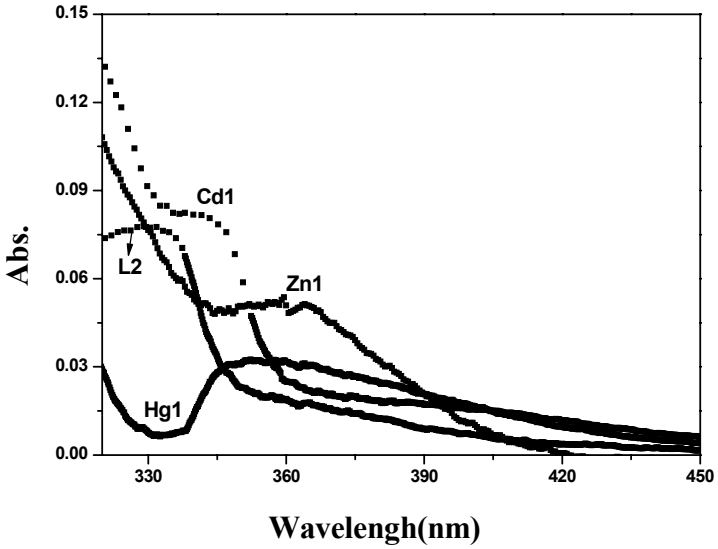

Fig. S3 UV-Vis absorption spectra of ligand and complexes 1–3.

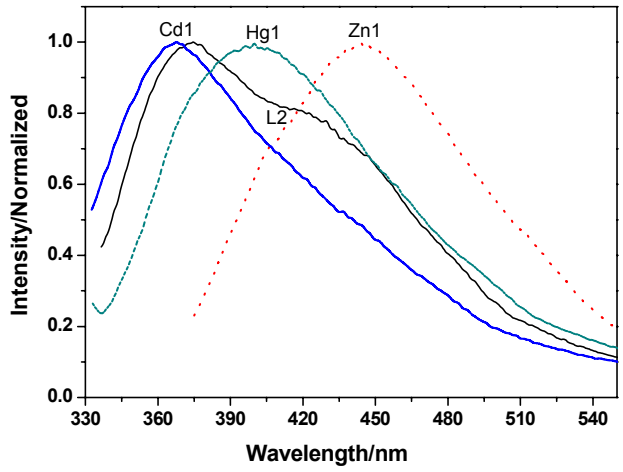

Fig. S4 Emission spectra of ligand and complexes 1–3 in CH_2Cl_2 solution at 298K. Concentration: [M] ≈ 10^{-5} M.

Table S5 Photoluminescent data for **Zn1**, **Cd1** and **Hg1**

compound	absorption (nm) ε/dm^3 mol^{-1} cm^{-1}	excitation (λ_{max}, nm)	emission (λ_{max}, nm)	conditions
Zn1	292(22850), 360(5491)		445	CH_2Cl_2, 298K
		330	484	solid, 298K
Cd1	305 (17195), 343 (8153)		399	CH_2Cl_2, 298K
		330	485	solid, 298K
Hg1	293(15590), 352(3221)		400	CH_2Cl_2, 298K
		330	486	solid, 298K