Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supporting Information

Mono-nuclear and di-nuclear photoluminescent complexes of zinc(II), cadmium(II) and mercury(II) of a chiral diimine ligand

*Suman Kundu, Suvendu Maity, Pinki Saha Sardar, Sanjib Ghosh, and Prasanta Ghosh**

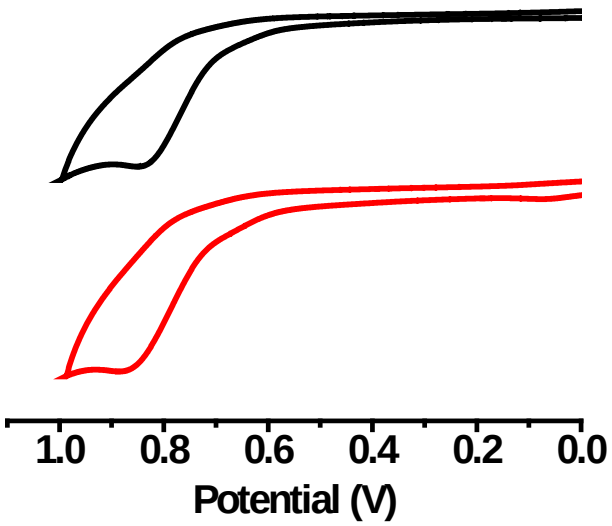

Fig. S1 Cyclic voltammograms of **1** in dichloromethane (black) and dimethylformamide (red) at 298 K. Conditions: 0.2 M $[N(n\text{-}Bu)_4]PF_6$ supporting electrolyte; scan rate: 100 mVs^{-1}; platinum working electrode.

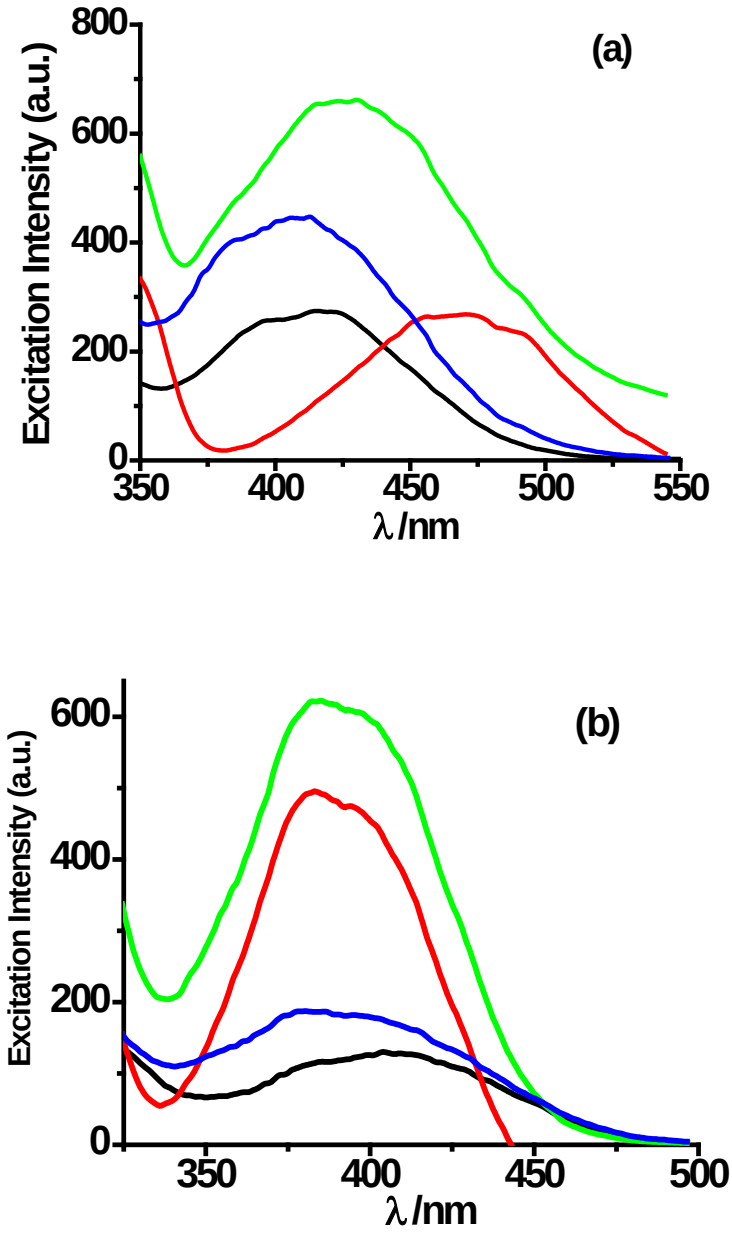

Fig. S2 Excitation spectra of **L** (black), **1** (red), **2** (green) and **3** (blue) in (**a**) CH_2Cl_2 and (**b**) CH_3CN solution at 298 K.

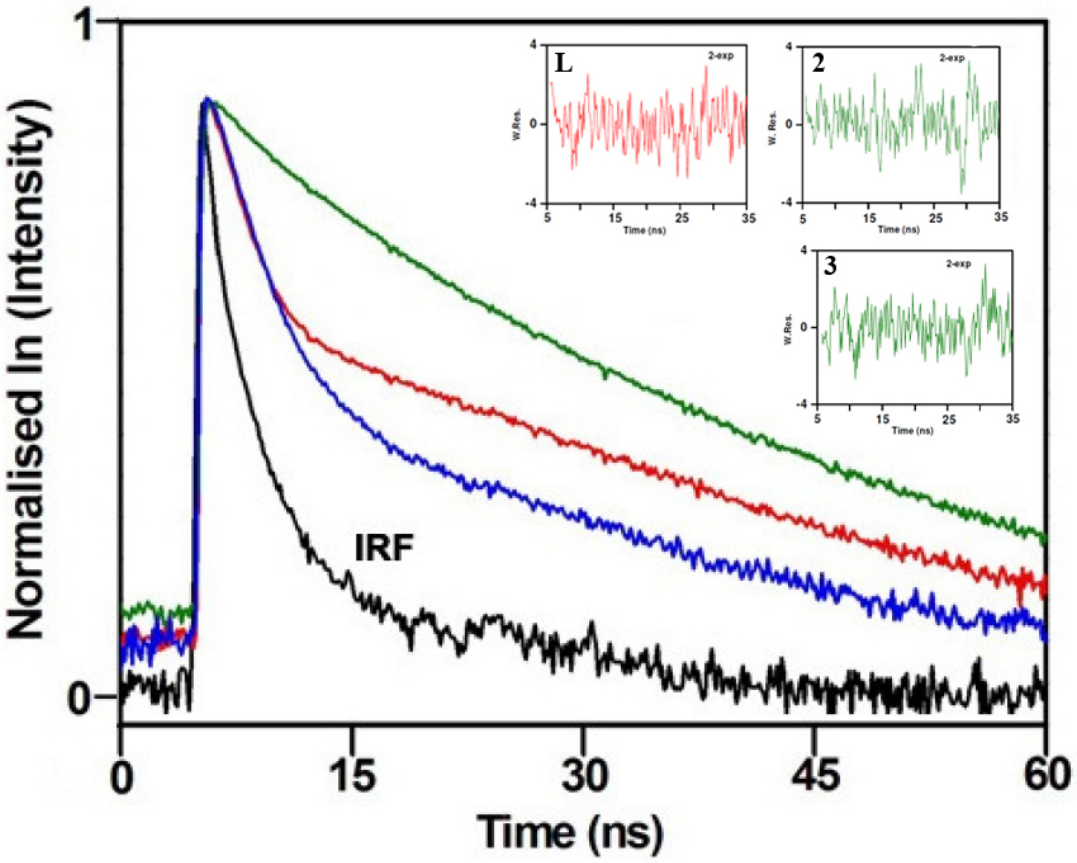

Fig. S3 Representative fluorescence decay (semi-log plot) of **L** (red), **2** (green), **3** (blue) in CH_2Cl_2 solution at 298 K.

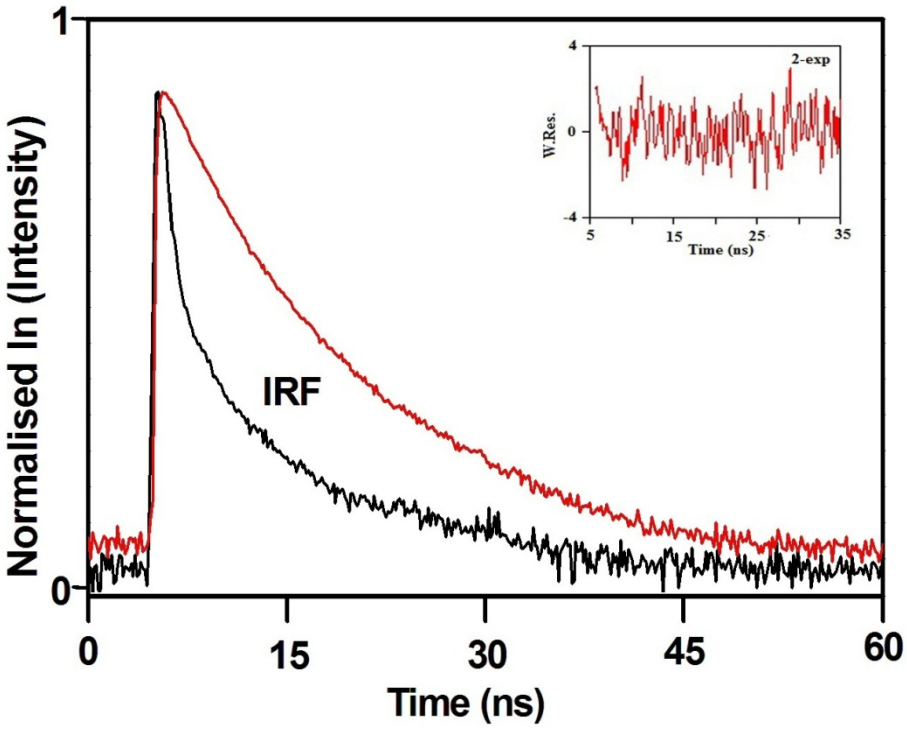

Fig. S4 Representative fluorescence decay (semi-log plot) of **1** in CH_2Cl_2 solution at 298 K.

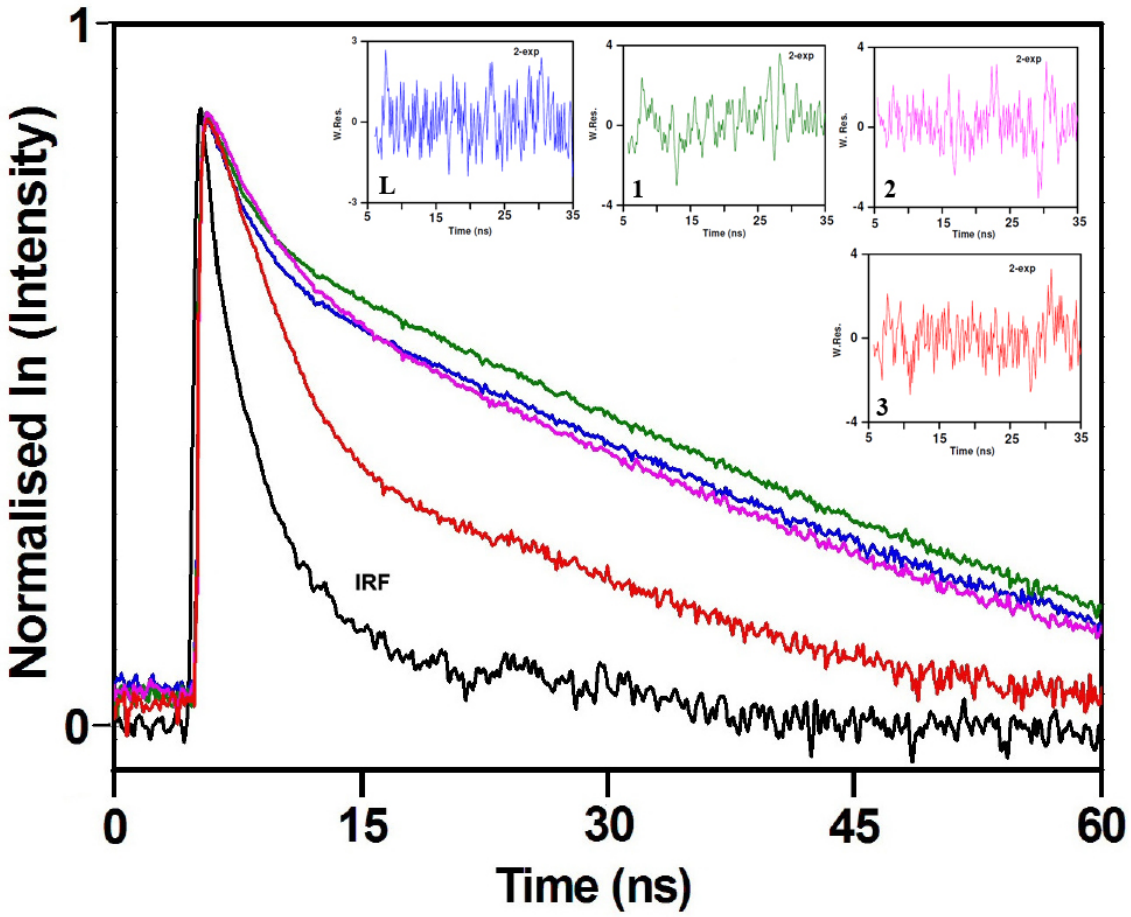

Fig. S5 Representative fluorescence decay (semi-log plot) of **L** (blue), **1** (green), **2** (pink) and **3** (red) in CH_3CN solution at 298 K.

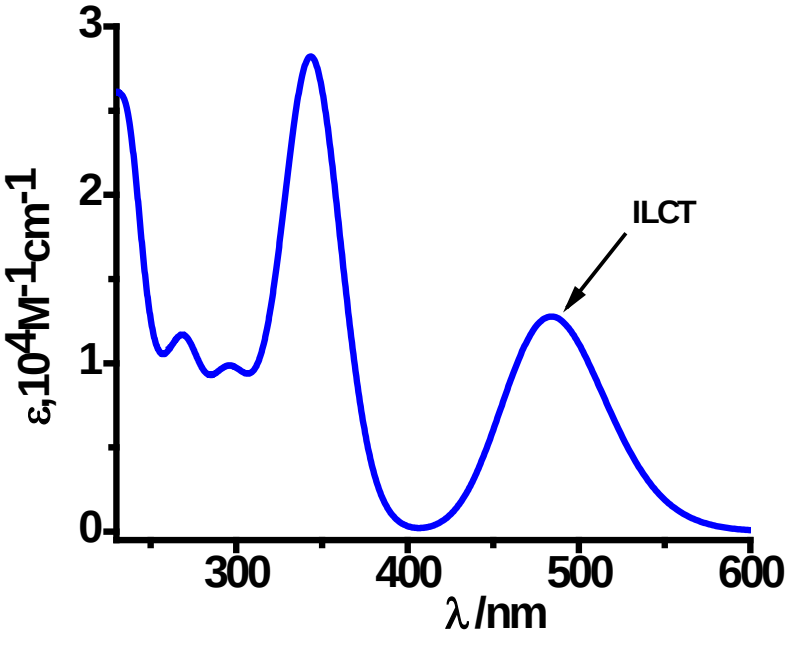

Fig. S6 Electronic absorption spectra of **1** obtained from TD DFT calculations in CH_2Cl_2.

Table S1 Excitation energies (λ/nm), oscillator strengths (f), transition types and dominant contributions of UV-vis absorption bands of **1** obtained from TD DFT calculations

λ_{cal}	f	λ_{exp}	Significant Transitions (>10%)	Dominant Contributions	Type
483	0.176	468	HOMO→LUMO (90)	L(91)→DI(78)+L(21)	ILCT
348	0.283	348	HOMO-1→LUMO (88)	X(99)→DI(78)+L(21)	XLCT
336	0.055	334	HOMO-3→LUMO (57) HOMO-2→LUMO (37)	X(83)+L(12)→DI(78)+L(21) X(94)→DI(78)+L(21)	XLCT XLCT
332	0.080		HOMO-3→LUMO (30) HOMO-2→LUMO (58)	X(83)+L(12)→DI(78)+L(21) X(94)→DI(78)+L(21)	XLCT XLCT
313	0.044		HOMO-5→LUMO (80)	X(30)+L(60)→DI(78)+L(21)	ILCT
296	0.022		HOMO-7→LUMO (16) HOMO-6→LUMO (30) HOMO→LUMO+2 (37)	L(99)→DI(78)+L(21) L(98) →DI(78)+L(21) L(91)→L(93)	ILCT ILCT ILCT
295	0.068		HOMO-7→LUMO (12) HOMO-6→LUMO (18) HOMO→LUMO+2 (55)	L(99) →DI(78)+L(21) L(98) →DI(78)+L(21) L(91)→L(93)	ILCT ILCT ILCT
286	0.012		HOMO→LUMO+3 (92)	L(91)→L(97)	ILCT
274	0.011	276	HOMO-10→LUMO (90)	X(96)→DI(78)+L(21)	XLCT

ILCT = Inter-Ligand Charge Transfer

XLCT = Halogen to Ligand Charge Transfer

X = Halogen (Cl)

DI = Diimines fragment of ligand $\mathbf{L}^{\mathbf{OMe}}$

L = Rest of the ligand $\mathbf{L}^{\mathbf{OMe}}$

Table S2 Gas phase optimized coordinates of [**1**] using B3LYP functionals

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	Zn	-2.353583	6.128858	6.689363	27	C	-3.517752	9.487882	11.705581
2	Cl	-3.491485	4.814763	5.251977	28	C	-2.687675	8.862468	12.646911
3	Cl	-0.563888	5.728318	8.049476	29	C	-2.498661	9.436783	13.903996
4	N	-2.104485	8.143535	5.922338	30	C	-3.125308	10.646396	14.224925
5	N	-3.560178	7.406345	8.057762	31	C	-3.941990	11.274381	13.281884
6	N	-3.704410	8.864127	10.420485	32	C	-4.146454	10.696831	12.024580
7	N	-1.896810	11.619300	9.565177	33	C	-5.576336	10.196565	8.588608
8	O	-4.245913	10.629852	8.876632	34	H	-1.275229	7.641721	4.103569
9	C	-1.586723	8.470427	4.733519	35	H	-1.027033	10.017504	3.341605
10	C	-1.452830	9.794336	4.314471	36	H	-1.804742	11.847567	4.887182
11	C	-1.883485	10.803043	5.175647	37	H	-2.789190	11.231372	7.090452
12	C	-2.429014	10.465840	6.414679	38	H	-0.884169	8.388373	9.524960
13	C	-2.526710	9.112010	6.766989	39	H	1.310894	9.465385	9.968126
14	C	-3.152296	8.635523	8.035565	40	H	1.412704	11.980027	10.161187
15	C	-3.312171	9.609501	9.215240	41	H	-0.708165	13.274747	9.876624
16	C	-1.945094	10.288278	9.482826	42	H	-4.757878	5.085989	8.086726
17	C	-0.815211	9.469454	9.621837	43	H	-6.018751	4.105328	10.006907
18	C	0.416670	10.074049	9.866019	44	H	-6.214305	5.410461	12.126792
19	C	0.475685	11.465205	9.969136	45	H	-5.166311	7.622033	12.347038
20	C	-0.708212	12.188135	9.810011	46	H	-2.197357	7.928639	12.386944
21	C	-4.345398	7.630018	10.345727	47	H	-1.854193	8.945014	14.627833
22	C	-4.245720	6.886342	9.146116	48	H	-2.974012	11.096459	15.202503
23	C	-4.846673	5.619682	9.029759	49	H	-4.427729	12.216627	13.521530
24	C	-5.552712	5.081532	10.095714	50	H	-4.772151	11.189514	11.289567
25	C	-5.658027	5.817990	11.286614	51	H	-6.134402	11.102546	8.342951
26	C	-5.068577	7.072384	11.418086	52	H	-6.036302	9.710683	9.457467
					53	H	-5.610252	9.510862	7.731385