Triazole linked anthracenyl-appended calix[4]arene conjugate for Co(II) recognition: by spectroscopy, microscopy and computational model

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Electronic Supporting Information

Contents Page No.

S1. Characterization of P_1

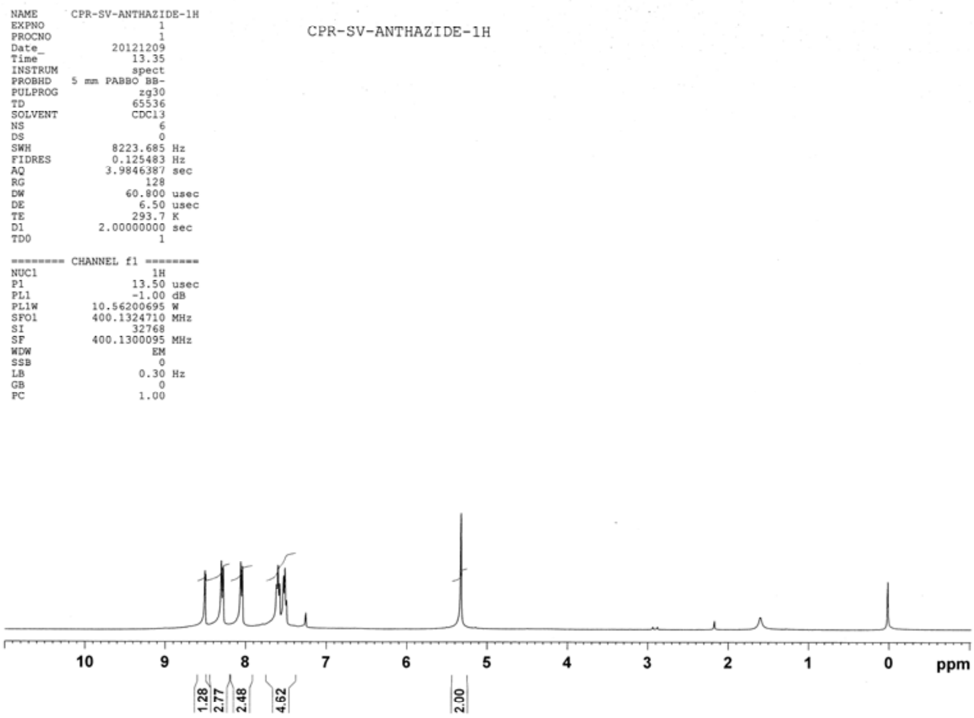


Figure S1: ^{1}H NMR spectra of P_1 in $CDCl_3$

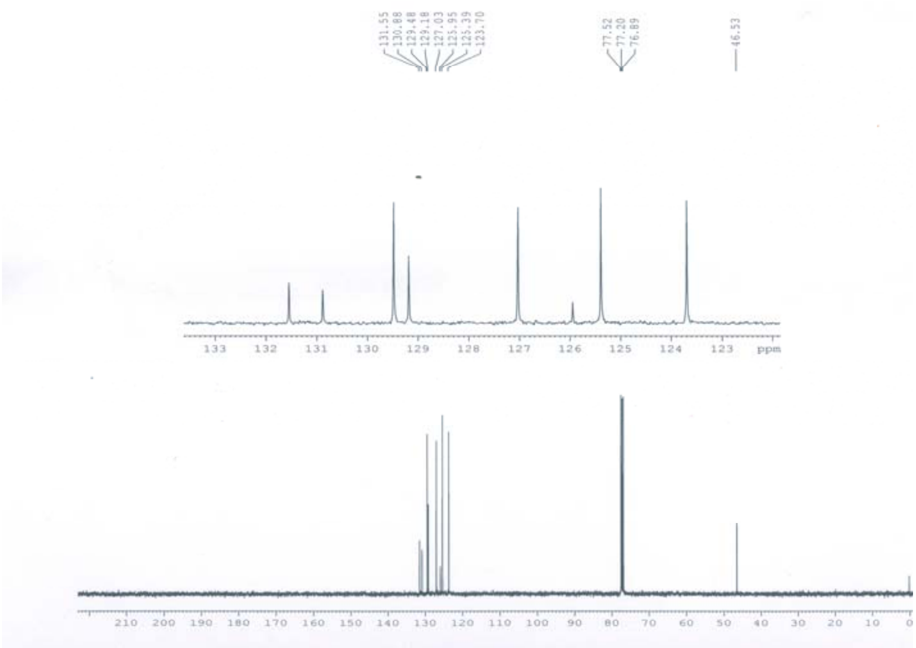


Figure S2: ^{13}C NMR spectra of P_1 in $CDCl_3$

Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 200.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Waters(Micromass) : Q-Tof micro(YA-105) Dept. Of Chemistry - I.I.T.(B) 03-Jan-201312:37:19
C15H11N3
CPR-ANTHRCENE-AZIDE 17 (0.168) AM (Cen,5, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 6x3.00); Sb (5,40.00); Cm (9:56) TOF MS ES+ 15.0

Minimum:				-1.5		
Maximum:		50.0	100.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
233.0957	233.0953	0.5	1.9	12.0	1	C15 H11 N3

Figure S3: HRMS spectrum of P_1

S2. Characterization of P_2

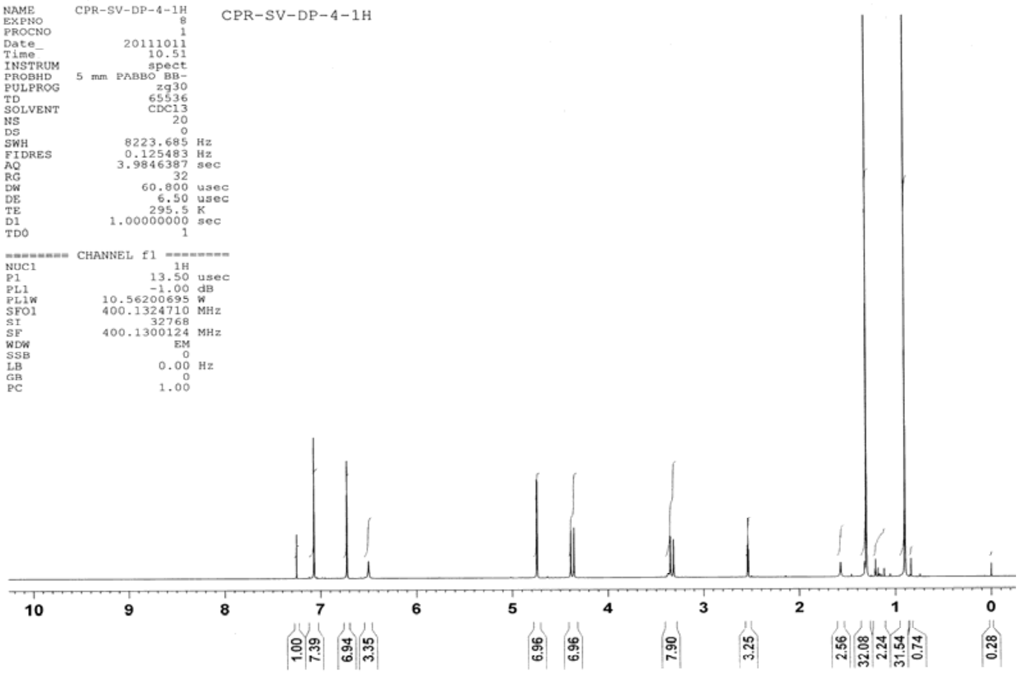


Figure S4: ^{1}H NMR spectra of P_2 in $CDCl_3$

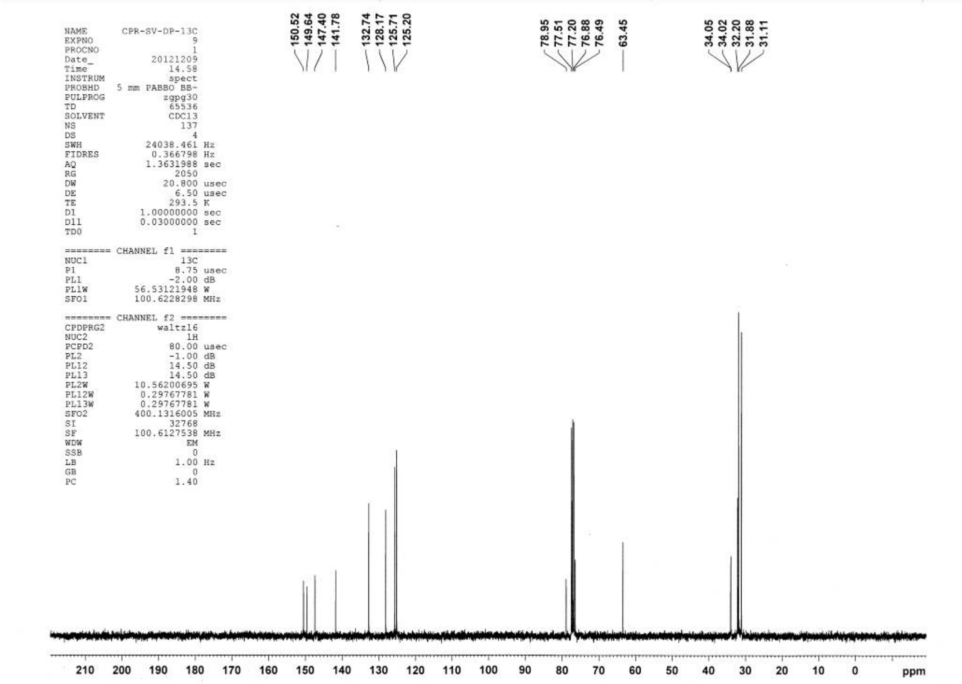


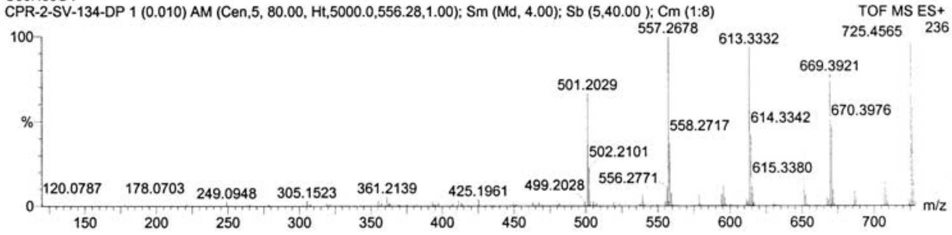
Figure S5: ^{13}C NMR spectra of P_2 in $CDCl_3$

Elemental Composition Report | **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 200.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Waters(Micromass) : Q-Tof micro(YA-105) Dept. Of Chemistry - I.I.T.(B) 19-Aug-201216:13:56
C50H60O4
CPR-2-SV-134-DP 1 (0.010) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Md, 4.00); Sb (5,40.00); Cm (1:8) TOF MS ES+



Minimum:				-1.5		
Maximum:		200.0	20.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
725.4565	725.4570	-0.5	-0.7	20.5	1	C50 H61 O4

Figure S6: HRMS spectrum of P_2

S3. Characterization of L

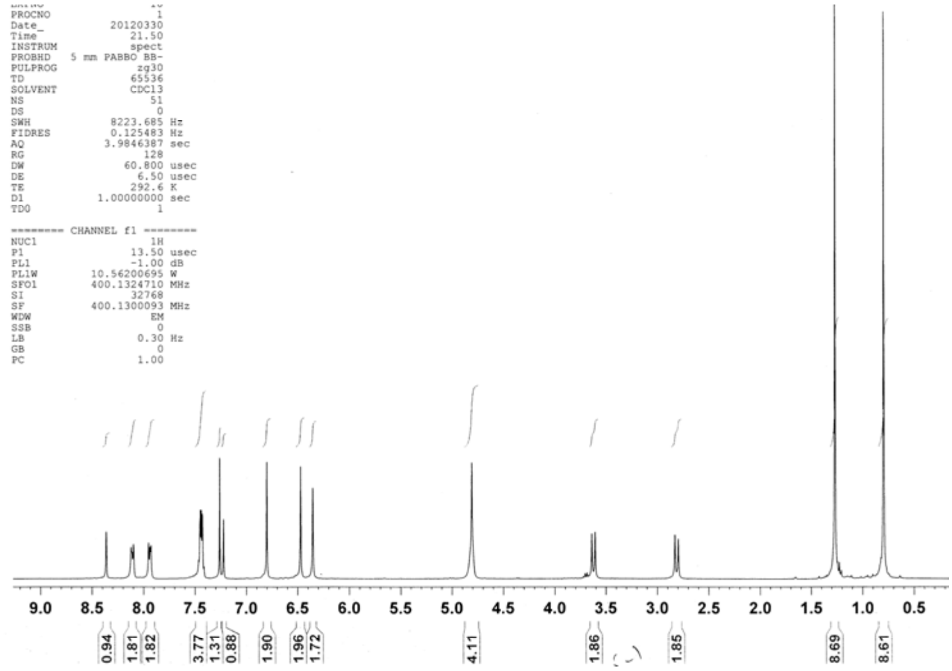


Figure S7: ^{1}H NMR spectra of **L** in $CDCl_3$

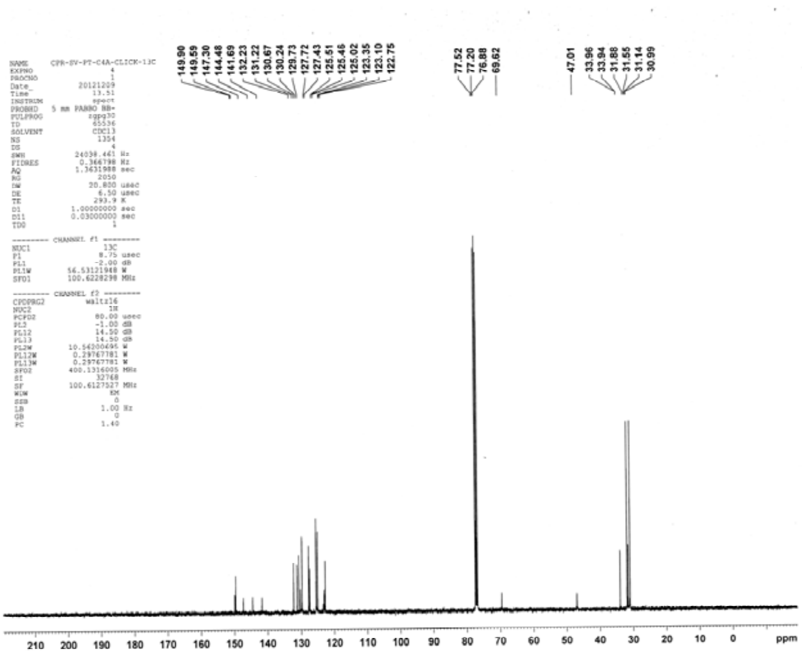


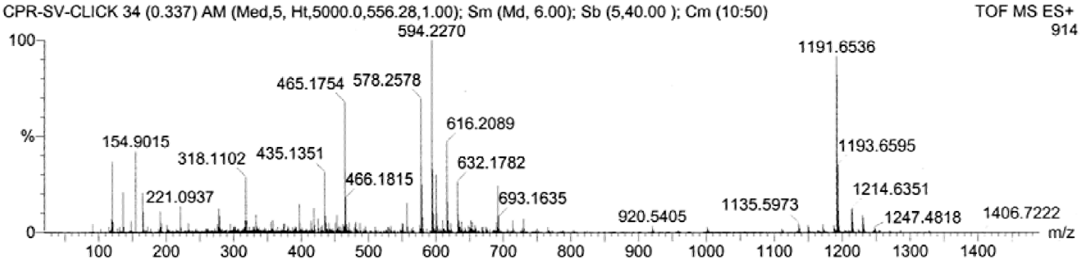
Figure S8: ^{13}C NMR spectra of L in $CDCl_3$

Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 09-Jan-201211:52:10
C80H82N6O4
CPR-SV-CLICK 34 (0.337) AM (Med,5, Ht,5000.0,556.28,1.00); Sm (Md, 6.00); Sb (5,40.00); Cm (10:50) TOF MS ES+ 914



Minimum:				-1.5		
Maximum:		200.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
1191.6536	1191.6476	6.0	5.0	42.5	1	C80 H83 N6 O4

Figure S9: HRMS spectrum for **L**

S4. Characterization of L_1

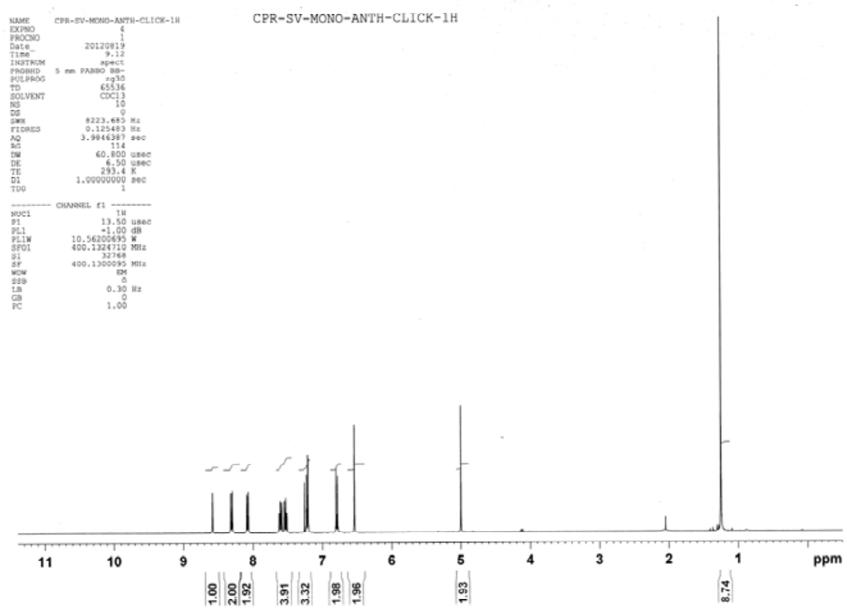


Figure S10: ^{1}H NMR spectra of L_1 in $CDCl_3$

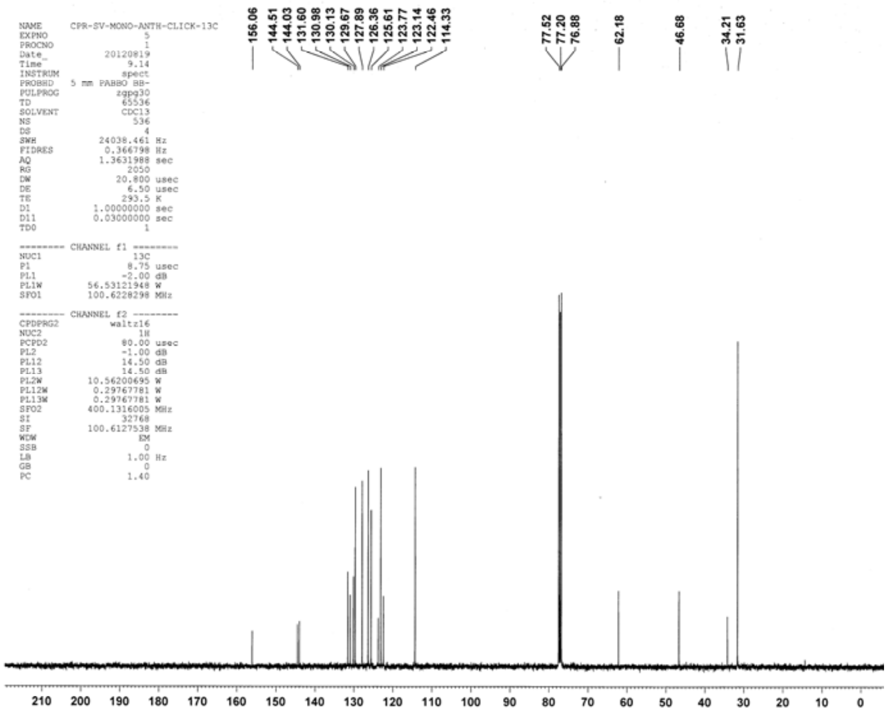


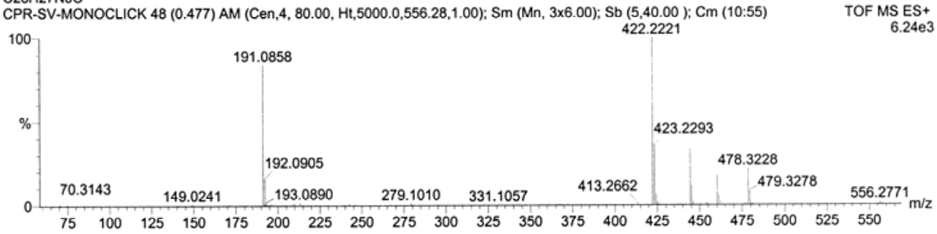
Figure S11: ^{13}C NMR spectra of L_1 in $CDCl_3$

Elemental Composition Report Page 1

Single Mass Analysis (displaying only valid results)
Tolerance = 15.0 PPM / DBE: min = -1.5, max = 200.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Waters(Micromass) : Q-Tof micro(YA-105) Dept. Of Chemistry - I.I.T.(B) 27-Dec-201222:03:00
C28H27N3O
CPR-SV-MONOCLICK 48 (0.477) AM (Cen,4, 80.00, Ht,5000.0,556.28,1.00); Sm (Mn, 3x6.00); Sb (5,40.00); Cm (10:55) TOF MS ES+
6.24e3



Minimum:				-1.5		
Maximum:		50.0	15.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
422.2221	422.2232	-1.1	-2.6	16.5	1	C28 H28 N3 O

Figure S12: HRMS spectrum for $\mathbf{L_1}$

S5. Preliminary crystallographic data for L

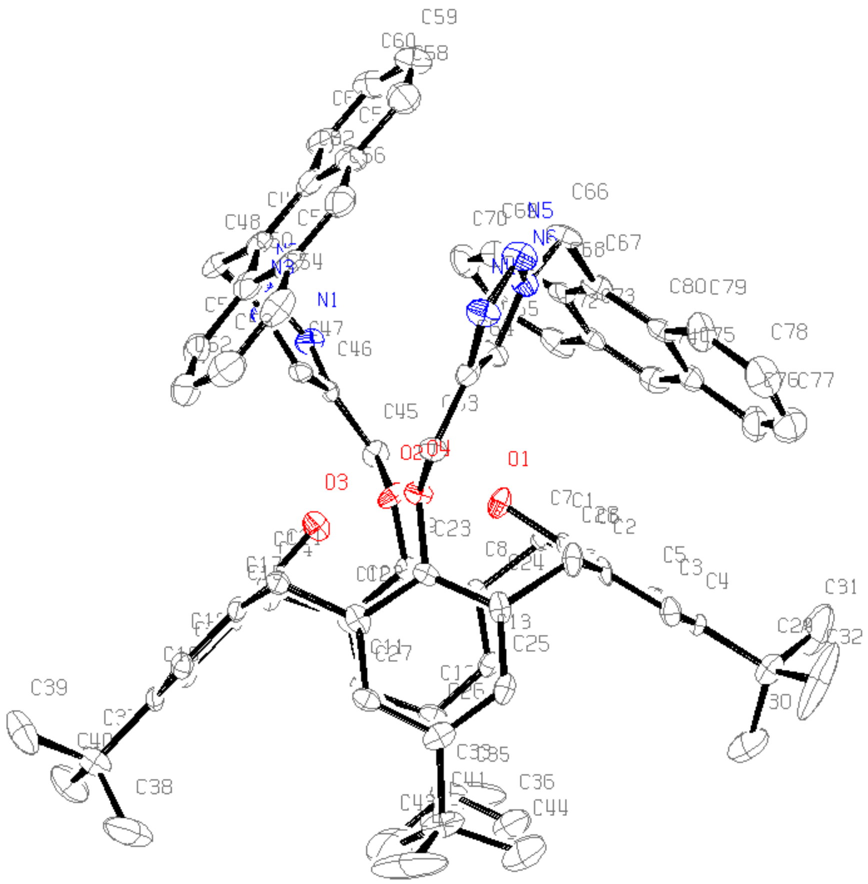


Figure S13: Single crystal structure of **L**

Table S1. **Crystallographic parameters for the structure determination and refinement**

	L
Empirical Formula	$C_{82}H_{84}Cl_6N_6O_4$
Molecular weight	1430.26
Temperature (K)	160
Crystal System	Triclinic
Space group	$P\bar{1}$ (No. 2)
a/Å	12.8268(14)
b/Å	16.8384(18)
c/Å	19.527(2)
α/°	70.017(6)
β/°	73.553(6)
γ/°	74.051(6)
Volume/$Å^3$	3726.5(7)
Z	2
Absorption coefficient (mu)	0.285
D_c/gcm^{-3}	1.275
Number of reflections	12858
R_{int}	0.067
Reflections used*	8766
Parameters	898
Final R	0.1034(8766)
wR_2	0.2368(12858)

Table S2 for bond distances

O1 - C1	1.370(6)	C15 - C20	1.391(7)
O1 - H1A	0.8400	C15 - C16	1.396(7)
O2 - C9	1.388(6)	C16 - C17	1.404(7)
O2 - C45	1.432(6)	C17 - C18	1.377(7)
O3 - C16	1.363(6)	C17 - C21	1.522(7)
O3 - H3A	0.8400	C18 - C19	1.389(7)
O4 - C23	1.394(6)	C18 - H18	0.9500
O4 - C63	1.442(6)	C19 - C20	1.391(7)
N1 - N2	1.322(6)	C19 - C37	1.540(7)
N1 - C46	1.356(6)	C20 - H20	0.9500
N2 - N3	1.341(6)	C21 - C22	1.513(7)
N3 - C47	1.337(6)	C21 – H21A	0.9900
N3 - C48	1.468(7)	C21 - H21B	0.9900
N4 - N5	1.326(6)	C22 - C27	1.386(7)
N4 - C64	1.358(7)	C22 - C23	1.399(7)
N5 - N6	1.349(6)	C23 - C24	1.399(7)
N6 - C65	1.343(7)	C24 - C25	1.393(7)
N6 - C66	1.473(7)	C24 - C28	1.522(7)
C1 - C6	1.401(7)	C25 - C26	1.390(8)
C1 - C2	1.401(7)	C25 - H25	0.9500
C2 - C3	1.385(7)	C26 - C27	1.400(7)
C2 - C28	1.516(7)	C26 - C41	1.532(8)
C3 - C4	1.378(7)	C27 - H27	0.9500
C3 - H3	0.9500	C28 - H28A	0.9900
C4 - C5	1.404(7)	C28 - H28B	0.9900
C4 - C29	1.542(7)	C29 - C32	1.513(9)
C5 - C6	1.397(7)	C29 - C31	1.520(9)
C5 - H5	0.9500	C29 - C30	1.524(9)
C6 - C7	1.508(7)	C30 - H30A	0.9800
C7 - C8	1.524(7)	C30 - H30B	0.9800
C7 - H7A	0.9900	C30 - H30C	0.9800
C7 - H7B	0.9900	C31 - H31A	0.9800
C8 - C9	1.387(7)	C31 - H31B	0.9800
C8 - C13	1.389(7)	C31 - H31C	0.9800
C9 - C10	1.398(7)	C32 - H32A	0.9800
C10 - C11	1.385(7)	C32 - H32B	0.9800
C10 - C14	1.521(7)	C32 - H32C	0.9800
C11 - C12	1.390(7)	C33 - C36	1.513(9)
C11 - H11	0.9500	C33 - C34	1.532(9)
C12 - C13	1.401(7)	C33 - C35	1.540(10
C12 - C33	1.536(7)	C34 - H34A	0.9800
C13 - H13	0.9500	C34 - H34B	0.9800

C14 - C15	1.526(7)	C34 - H34C	0.9800
C14 - H14A	0.9900	C35 - H35A	0.9800
C14 - H14B	0.9900	C35 - H35B	0.9800
C35 - H35C	0.9800	C53 - H53	0.9500
C36 - H36A	0.9800	C54 - C55	1.417(8)
C36 - H36B	0.9800	C54 - H54	0.9500
C36 - H36C	0.9800	C55 - C56	1.392(8)
C37 - C40	1.524(8)	C56 - C57	1.431(8)
C37 - C38	1.531(9)	C56 - H56	0.9500
C37 - C39	1.548(9)	C57 - C62	1.409(8)
C38 - H38A	0.9800	C57 - C58	1.419(8)
C38 - H38B	0.9800	C58 - C59	1.382(9)
C38 - H38C	0.9800	C58 - H58	0.9500
C39 - H39A	0.9800	C59 - C60	1.398(9)
C39 - H39B	0.9800	C59 - H59	0.9500
C39 - H39C	0.9800	C60 - C61	1.355(9)
C40 - H40A	0.9800	C60 - H60	0.9500
C40 - H40B	0.9800	C61 - C62	1.428(8)
C40 - H40C	0.9800	C61 - H61	0.9500
C41 - C44	1.510(10)	C63 - C64	1.483(7)
C41 - C42	1.510(10)	C63 - H63A	0.9900
C41 - C43	1.541(10)	C63 - H63B	0.9900
C42 - H42A	0.9800	C64 - C65	1.362(7)
C42 - H42B	0.9800	C65 - H65	0.9500
C42 - H42C	0.9800	C66 - C67	1.516(8)
C43 - H43A	0.9800	C66 - H66A	0.9900
C43 - H43B	0.9800	C66 - H66B	0.9900
C43 - H43C	0.9800	C67 - C80	1.401(8)
C44 - H44A	0.9800	C67 - C68	1.420(8)
C44 - H44B	0.9800	C68 - C73	1.428(8)
C44 - H44C	0.9800	C68 - C69	1.444(8)
C45 - C46	1.495(7)	C69 - C70	1.351(8)
C45 - H45A	0.9900	C69 - H69	0.9500
C45 - H45B	0.9900	C70 - C71	1.392(9)
C46 - C47	1.369(7)	C70 - H70	0.9500
C47 - H47	0.9500	C71 - C72	1.365(9)
C48 - C49	1.521(8)	C71 - H71	0.9500
C48 - H48A	0.9900	C72 - C73	1.437(8)
C48 - H48B	0.9900	C72 - H72	0.9500
C49 - C50	1.407(8)	C73 - C74	1.381(8)
C49 - C62	1.417(8)	C74 - C75	1.406(8)
C50 - C55	1.438(8)	C74 - H74	0.9500
C50 - C51	1.442(8)	C75 - C76	1.419(8)
C51 - C52	1.353(9)	C75 - C80	1.442(8)
C51 - H51	0.9500	C76 - C77	1.370(9)

C52 - C53	1.430(9)	C76 - H76	0.9500
C52 - H52	0.9500	C77 - C78	1.398(9)
C53 - C54	1.344(9)	C77 - H77	0.9500
C78 - C79	1.337(9)	C81 - H81	1.0000
C78 - H78	0.9500	C82 - Cl6	1.739(7)
C79 - C80	1.439(8)	C82 - Cl4	1.750(7)
C79 - H79	0.9500	C82 - Cl5	1.757(7)
C81 - Cl2	1.746(7)	C82 - H82	1.0000
C81 - Cl1	1.752(6)	C78 - C79	1.337(9)
C81 - Cl3	1.754(6)	C78 - H78	0.9500
C79 - H79	0.9500	C79 - C80	1.439(8)
C81 - Cl2	1.746(7)	C82 - Cl6	1.739(7)
C81 - Cl1	1.752(6)	C82 - Cl4	1.750(7)
C81 - Cl3	1.754(6)	C82 - Cl5	1.757(7)
C81 - H81	1.0000	C82 - H82	1.0000

Table S3 for bond angles

C1 - O1 - H1A	109.5	C11 - C12 - C13	116.8(5)
C9 - O2 - C45	114.1(4)	C11 - C12 - C33	123.4(5)
C16 - O3 - H3A	109.5	C13 - C12 - C33	119.8(5)
C23 - O4 - C63	115.4(4)	C8 - C13 - C12	122.9(5)
N2 - N1 - C46	108.6(4)	C8 - C13 - H13	118.5
N1 - N2 - N3	107.2(4)	C12 - C13 - H13	118.5
C47 - N3 - N2	110.8(4)	C10 - C14 - C15	112.7(4)
C47 - N3 - C48	129.3(5)	C10 - C14 - H14A	109.1
N2 - N3 - C48	119.9(4)	C15 - C14 - H14A	109.1
N5 - N4 - C64	108.2(4)	C10 - C14 - H14B	109.1
N4 - N5 – N6	106.7(4)	C15 - C14 - H14B	109.1
C65 - N6 - N5	111.4(4)	H14A - C14 - H14B	107.8
C65 - N6 - C66	128.5(4)	C20 - C15 - C16	119.2(5)
N5 - N6 - C66	120.0(4)	C20 - C15 - C14	120.0(5)
O1 - C1 - C6	119.1(4)	C16 - C15 - C14	120.8(5)
O1 - C1 - C2	120.4(4)	O3 - C16 - C15	120.7(5)
C6 - C1 - C2	120.5(4)	O3 - C16 - C17	119.4(5)
C3 - C2 - C1	118.8(5)	C15 - C16 - C17	119.9(5)
C3 - C2 - C28	121.2(5)	C18 - C17 - C16	118.4(5)
C1 - C2 - C28	119.9(4)	C18 - C17 - C21	122.2(5)
C4 - C3 - C2	123.0(5)	C16 - C17 - C21	118.8(4)
C4 - C3 - H3	118.5	C17 - C18 – C19	123.8(5)
C2 - C3 - H3	118.5	C17 - C18 - H18	118.1
C3 - C4 - C5	117.0(4)	C19 - C18 - H18	118.1
C3 - C4 - C29	122.7(5)	C18 - C19 - C20	116.4(5)
C5 - C4 - C29	120.3(5)	C18 - C19 - C37	120.2(5)
C6 - C5 - C4	122.4(5)	C20 - C19 - C37	123.4(5)
C6 - C5 - H5	118.8	C15 - C20 - C19	122.4(5)
C4 - C5 - H5	118.8	C15 - C20 - H20	118.8
C5 - C6 - C1	118.2(5)	C19 - C20 - H20	118.8
C5 - C6 - C7	121.2(5)	C22 - C21 - C17	109.0(4)
C1 - C6 - C7	120.4(4)	C22 - C21 - H21A	109.9
C6 - C7 - C8	110.7(4)	C17 - C21 - H21A	109.9
C6 - C7 - H7A	109.5	C22 - C21 - H21B	109.9
C8 - C7 - H7A	109.5	C17 - C21 - H21B	109.9
C6 - C7 - H7B	109.5	H21A - C21 - H21B	108.3
C8 - C7 - H7B	109.5	C27 - C22 - C23	117.6(5)
H7A - C7 - H7B	108.1	C27 - C22 - C21	120.4(5)
C9 - C8 - C13	117.8(4)	C23 - C22 - C21	121.8(4)
C9 - C8 - C7	122.3(4)	O4 - C23 - C22	118.4(4)
C13 - C8 - C7	119.7(4)	O4 - C23 - C24	119.4(4)
C8 - C9 - O2	119.6(4)	C22 - C23 - C24	121.9(5)
C8 - C9 - C10	121.5(4)	C25 - C24 - C23	117.9(5)

O2 - C9 - C10	118.9(4)	C25 - C24 - C28	119.6(5)
C11 - C10 - C9	118.5(5)	C23 - C24 - C28	122.4(5)
C11 - C10 - C14	120.1(5)	C26 - C25 - C24	122.4(5)
C9 - C10 - C14	121.4(5)	C26 - C25 - H25	118.8
C10 - C11 - C12	122.4(5)	C24 - C25 - H25	118.8
C10 - C11 - H11	118.8	C25 - C26 - C27	117.3(5)
C12 - C11 - H11	118.8	C25 - C26 - C41	123.3(5)
C27 - C26 - C41	119.5(5)	H35A - C35 - H35C	109.5
C22 - C27 - C26	122.9(5)	H35B - C35 - H35C	109.5
C22 - C27 - H27	118.6	C33 - C36 - H36A	109.5
C26 - C27 - H27	118.6	C33 - C36 - H36B	109.5
C2 - C28 - C24	111.0(4)	H36A - C36 - H36B	109.5
C2 - C28 - H28A	109.4	C33 - C36 - H36C	109.5
C24 - C28 - H28A	109.4	H36A - C36 - H36C	109.5
C2 - C28 - H28B	109.4	H36B - C36 - H36C	109.5
C24 - C28 - H28B	109.4	C40 - C37 - C38	110.1(5)
H28A - C28 - H28B	108.0	C40 - C37 - C19	112.1(5)
C32 - C29 - C31	107.4(7)	C38 - C37 - C19	108.6(5)
C32 - C29 - C30	108.9(7)	C40 - C37 - C39	107.3(5)
C31 - C29 - C30	108.6(6)	C38 - C37 - C39	109.9(6)
C32 - C29 - C4	112.1(5)	C19 - C37 - C39	108.8(5)
C31 C29 C4	110.9(5)	C37 - C38 - H38A	109.5
C30 - C29 - C4	108.8(5)	C37 - C38 - H38B	109.5
C29 - C30 - H30A	109.5	H38A - C38 - H38B	109.5
C29 - C30 - H30B	109.5	C37 - C38 – H38C	109.5
H30A - C30 - H30B	109.5	H38A - C38 - H38C	109.5
C29 - C30 - H30C	109.5	H38B - C38 - H38C	109.5
H30A - C30 - H30C	109.5	C37 - C39 - H39A	109.5
H30B - C30 - H30C	109.5	C37 - C39 - H39B	109.5
C29 - C31 - H31A	109.5	H39A - C39 - H39B	109.5
C29 - C31 - H31B	109.5	C37 - C39 - H39C	109.5
H31A - C31 - H31B	109.5	H39A - C39 - H39C	109.5
C29 - C31 - H31C	109.5	H39B - C39 - H39C	109.5
H31A - C31 - H31C	109.5	C37 - C40 - H40A	109.5
H31B - C31 - H31C	109.5	C37 - C40 - H40B	109.5
C29 - C32 - H32A	109.5	H40A - C40 - H40B	109.5
C29 - C32 - H32B	109.5	C37 - C40 - H40C	109.5
H32A - C32 - H32B	109.5	H40A - C40 - H40C	109.5
C29 - C32 - H32C	109.5	H40B - C40 - H40C	109.5
H32A - C32 - H32C	109.5	C44 - C41 - C42	110.0(7)
H32B - C32 - H32C	109.5	C44 - C41 - C26	112.1(6)
C36 - C33 - C34	106.7(5)	C42 - C41 - C26	109.8(5)
C36 - C33 - C12	111.6(5)	C44 - C41 - C43	108.3(7)
C34 - C33 - C12	112.3(5)	C42 - C41 - C43	107.7(7)
C36 - C33 - C35	109.2(7)	C26 - C41 - C43	108.7(5)
C34 - C33 - C35	108.3(7)	C41 - C42 - H42A	109.5

C12 - C33 - C35	108.6(5)	C41 - C42 - H42B	109.5
C33 - C34 - H34A	109.5	H42A - C42 - H42B	109.5
C33 - C34 - H34B	109.5	C41 - C42 - H42C	109.5
H34A - C34 - H34B	109.5	H42A - C42 - H42C	109.5
C33 - C34 - H34C	109.5	H42B - C42 - H42C	109.5
H34A - C34 - H34C	109.5	C41 - C43 - H43A	109.5
H34B - C34 - H34C	109.5	C41 - C43 - H43B	109.5
C33 - C35 - H35A	109.5	H43A - C43 - H43B	109.5
C33 - C35 - H35B	109.5	C41 - C43 - H43C	109.5
H35A - C35 - H35B	109.5	H43A - C43 - H43C	109.5
C33 - C35 - H35C	109.5	H43B - C43 - H43C	109.5
C41 - C44 - H44A	109.5	C58 - C57 - C56	119.6(6)
C41 - C44 - H44B	109.5	C59 - C58 - C57	119.5(6)
H44A - C44 - H44B	109.5	C59 - C58 - H58	120.3
C41 - C44 - H44C	109.5	C57 - C58 - H58	120.3
H44A - C44 - H44C	109.5	C58 - C59 - C60	119.9(6)
H44B - C44 - H44C	109.5	C58 - C59 - H59	120.1
O2 - C45 - C46	108.3(4)	C60 - C59 - H59	120.1
O2 - C45 - H45A	110.0	C61 - C60 - C59	121.2(6)
C46 - C45 - H45A	110.0	C61 - C60 - H60	119.4
O2 - C45 - H45B	110.0	C59 - C60 - H60	119.4
C46 - C45 - H45B	110.0	C60 - C61 - C62	121.4(6)
H45A - C45 - H45B	108.4	C60 - C61 - H61	119.3
N1 - C46 - C47	108.1(4)	C62 - C61 - H61	119.3
N1 - C46 - C45	121.8(4)	C57 - C62 - C49	120.3(5)
C47 - C46 - C45	130.1(4)	C57 - C62 - C61	117.0(6)
N3 - C47 - C46	105.3(4)	C49 - C62 - C61	122.6(6)
N3 - C47 - H47	127.4	O4 - C63 - C64	107.4(4)
C46 - C47 - H47	127.4	O4 - C63 - H63A	110.2
N3 - C48 - C49	111.2(4)	C64 - C63 - H63A	110.2
N3 - C48 - H48A	109.4	O4 - C63 - H63B	110.2
C49 - C48 - H48A	109.4	C64 - C63 - H63B	110.2
N3 - C48 - H48B	109.4	H63A - C63 - H63B	108.5
C49 - C48 - H48B	109.4	N4 - C64 - C65	109.4(5)
H48A - C48 - H48B	108.0	N4 - C64 - C63	122.7(5)
C50 - C49 - C62	120.0(5)	C65 - C64 - C63	127.8(5)
C50 - C49 - C48	120.3(5)	N6 - C65 - C64	104.3(4)
C62 - C49 - C48	119.7(5)	N6 - C65 - H65	127.9
C49 - C50 - C55	120.0(5)	C64 - C65 - H65	127.9
C49 - C50 - C51	122.9(6)	N6 - C66 - C67	110.6(4)
C55 - C50 - C51	117.15)	N6 - C66 - H66A	109.5
C52 - C51 - C50	121.3(6)	C67 - C66 - H66A	109.5
C52 - C51 - H51	119.3	N6 - C66 - H66B	109.5
C50 - C51 - H51	119.3	C67 - C66 - H66B	109.5
C51 - C52 - C53	120.5(6)	H66A - C66 - H66B	108.1
C51 - C52 - H52	119.8	C80 - C67 - C68	120.2(5)

C53 - C52 - H52	119.8	C80 - C67 - C66	119.1(5)
C54 - C53 - C52	120.1(6)	C68 - C67 - C66	120.6(5)
C54 - C53 - H53	119.9	C67 - C68 - C73	119.6(5)
C52 - C53 - H53	119.9	C67 - C68 - C69	122.9(5)
C53 - C54 - C55	121.6(6)	C73 - C68 - C69	117.5(5)
C53 - C54 - H54	119.2	C70 - C69 - C68	121.0(6)
C55 - C54 - H54	119.2	C70 - C69 - H69	119.5
C56 - C55 - C54	121.2(6)	C68 - C69 - H69	119.5
C56 - C55 - C50	119.5(6)	C69 - C70 - C71	121.7(6)
C54 - C55 - C50	119.4(6)	C69 - C70 - H70	119.1
C55 - C56 - C57	120.8(6)	C71 - C70 - H70	119.1
C55 - C56 - H56	119.6	C72 - C71 - C70	120.1(6)
C57 - C56 - H56	119.6	C72 - C71 - H71	120.0
C62 - C57 - C58	121.0(6)	C70 - C71 - H71	120.0
C62 - C57 - C56	119.4(5)	C71 - C72 - C73	120.9(6)
C71 - C72 - H72	119.5	C77 - C76 - C75	120.8(6)
C73 - C72 - H72	119.5	C77 - C76 - H76	119.6
C74 - C73 - C68	119.7(5)	C75 - C76 - H76	119.6
C74 - C73 - C72	121.5(5)	C76 - C77 - C78	119.9(6)
C68 - C73 - C72	118.7(5)	C76 - C77 - H77	120.0
C73 - C74 - C75	121.8(5)	C78 - C77 - H77	120.0
C73 - C74 - H74	119.1	C79 - C78 - C77	121.3(6)
C75 - C74 - H74	119.1	C79 - C78 - H78	119.3
C74 - C75 - C76	121.7(5)	C77 - C78 - H78	119.3
C74 - C75 - C80	118.9(5)	C78 - C79 - C80	122.2(6)
C76 - C75 - C80	119.4(5)	C78 - C79 - H79	118.9
C80 - C79 - H79	118.9	Cl3 - C81 - H81	108.2
C67 - C80 - C79	124.0(5)	Cl6 - C82 - Cl4	109.7(4)
C67 - C80 - C75	119.7(5)	Cl6 - C82 - Cl5	110.1(4)
C79 - C80 - C75	116.3(5)	Cl4 - C82 - Cl5	111.4(4)
Cl2 - C81 - Cl1	110.0(3)	Cl6 - C82 - H82	108.5
Cl2 - C81 - Cl3	111.4(3)	Cl4 - C82 - H82	108.5
Cl1 - C81 - Cl3	110.7(3)	Cl5 - C82 - H82	108.5
Cl2 - C81 - H81	108.2	Cl1 - C81 - H81	108.2

S6. Fluorescence studies of L with different metal ions

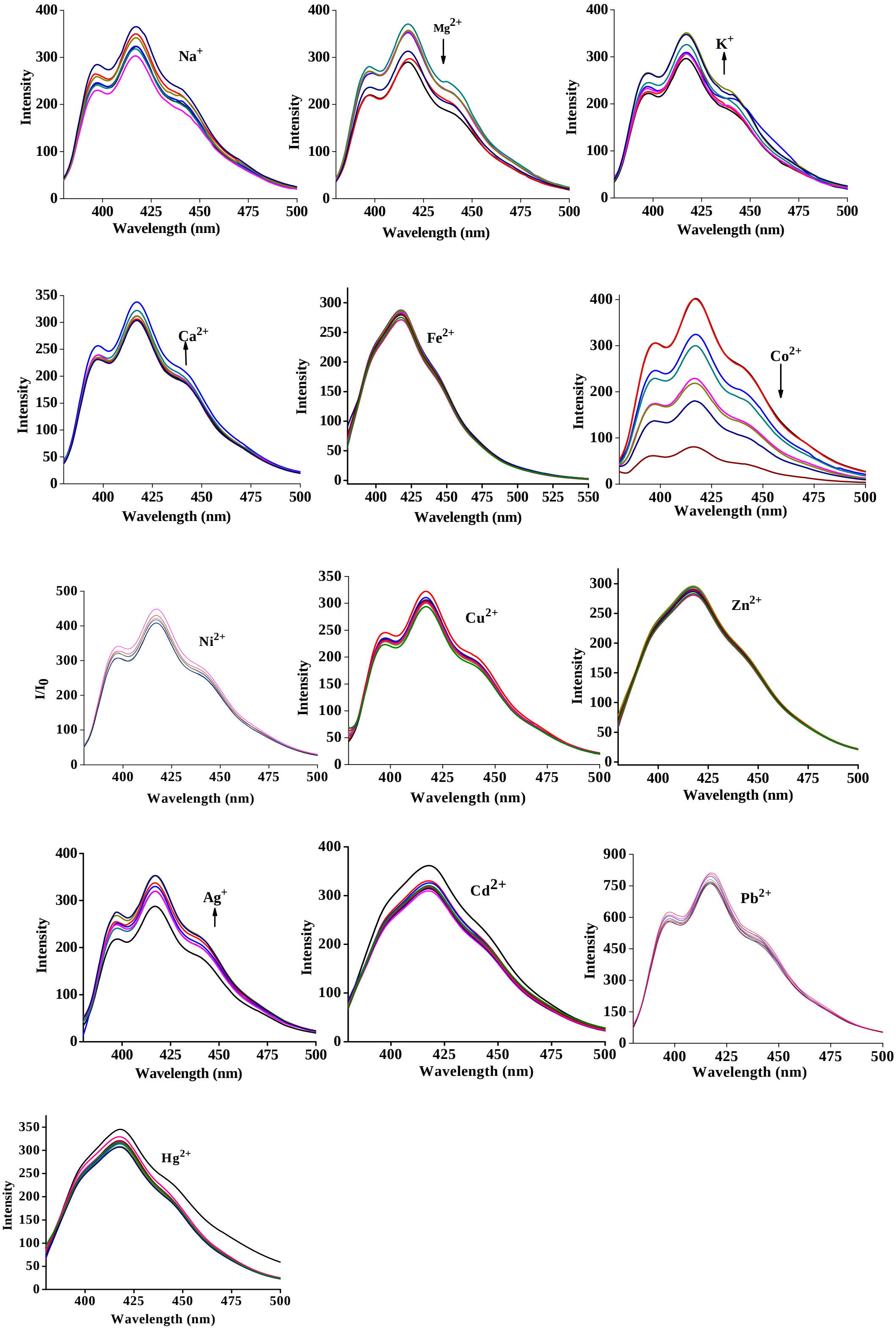


Figure S14: Fluorescence studies of **L** with different metal ions

S7. **Dilution experiment by maintaining the ratio of L:Co^{2+} as 1:1**

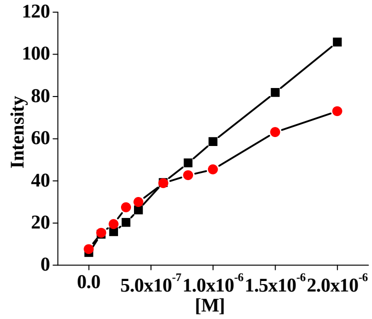


Figure S15: Determination of minimum concentration of Co^{2+} that can be detected by **L**.

S8: **Association constant of {L.Co^{2+}}**

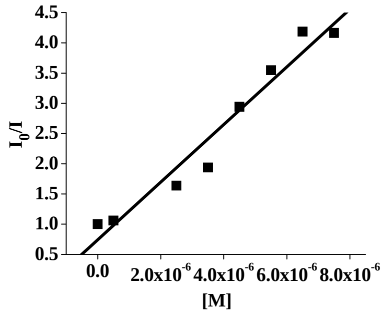


Figure S16: Determination of Stern – Volmer quenching constant for {**L**.Co^{2+}}.

S9. Absorbance studies of L with different metal ions

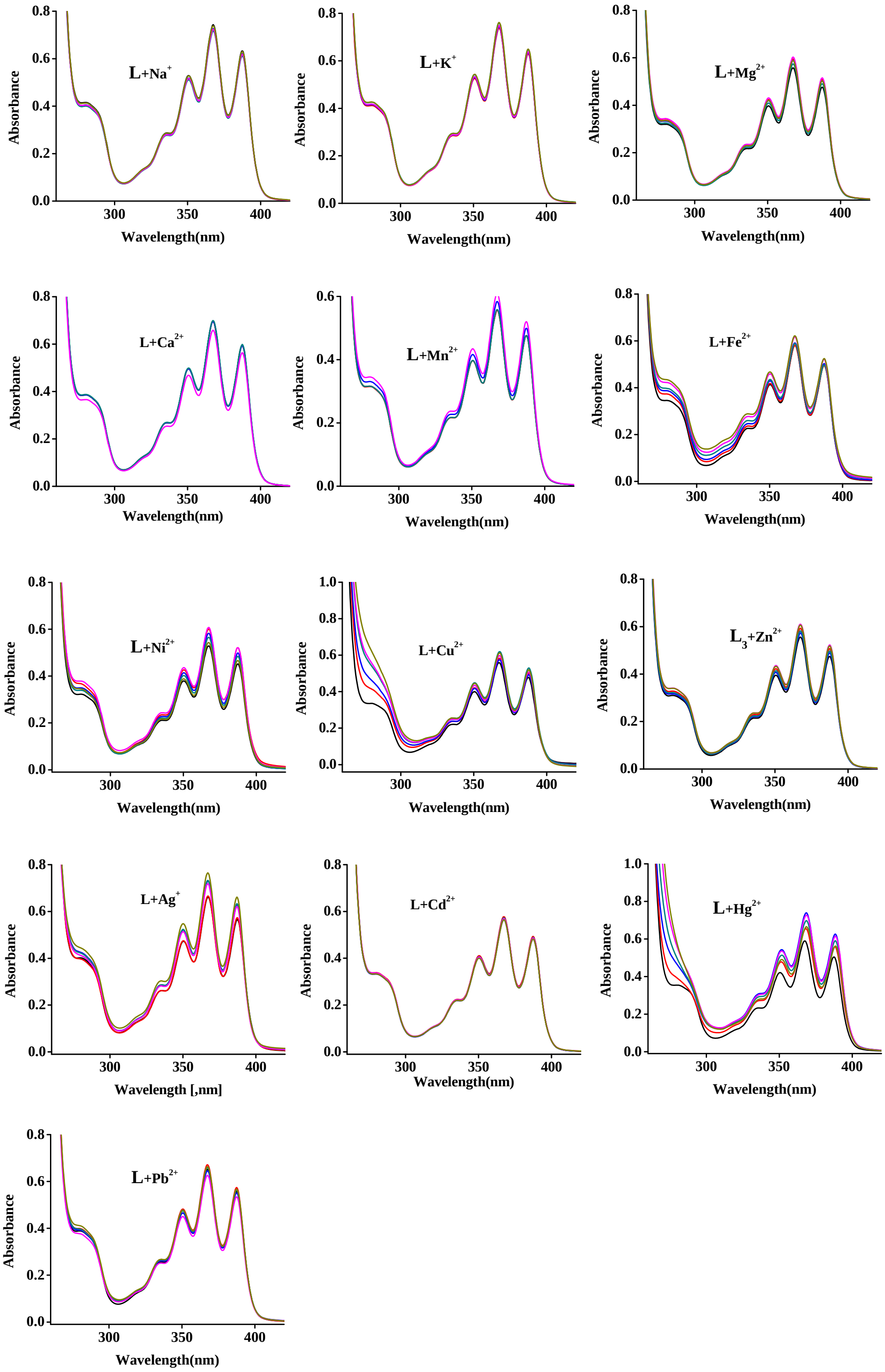


Figure S17: Absorbance studies of **L** with different metal ions

S10. ^{1}H NMR titration of L and L_1 with Co^{2+} ion:

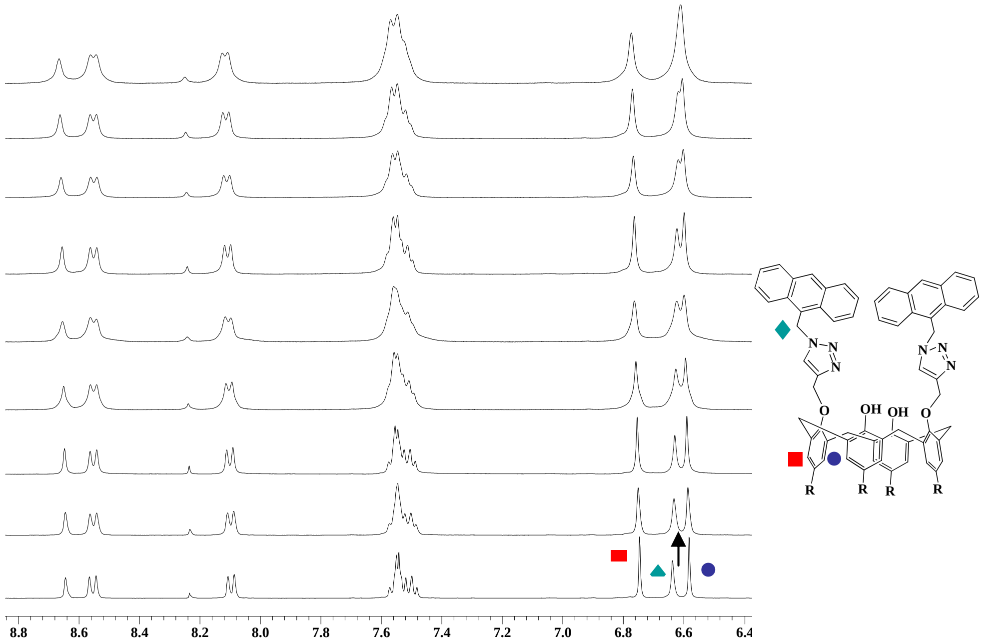


Figure S18: ^{1}H NMR titration of **L** with Co^{2+} ion

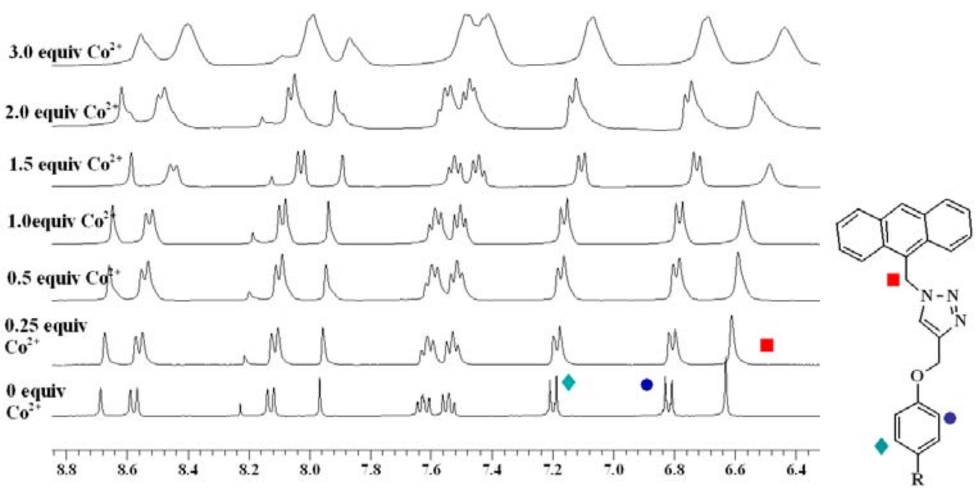


Figure S19: ^{1}H NMR titration of $\mathbf{L}_1$ with Co^{2+} ion

S11. Size distribution histogram for L and {L + Co^{2+}} by AFM and TEM:

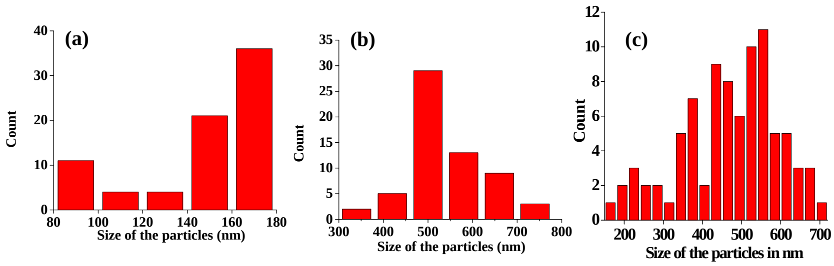


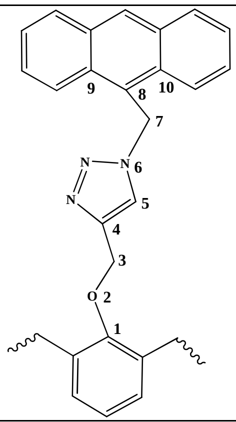
Figure S20: Size distribution histograms for **L** and {**L**+ Co^{2+}} are (a) & (b) respectively from AFM images. (c) Size distribution histogram for **L** based on TEM images.

S12 Computational data

Table S4: Table of dihedral angle (°) variation in case of complexed and uncomplexed [**L**.Co^{2+}] system.

System		**1–2–3–4**	**2–3–4–5**	**3–4–5–6**	**4–5–6–7**	**5–6–7–8**	**2-3-4-10**	**5-6-7-9**
L_1	**Arm1**	141.2	-15.3	-176.5	177.4	64.1	-104.7	77.3
	Arm2	138.0	-4.1	-178.9	-177.3	-49.7	-70.9	111.5
CoL_1	**Arm1**	-126.5	166.3	179.4	179.9	-30.8	105.6	-75.7
	Arm2	-126.5	166.3	179.3	179.9	-30.7	105.5	-75.8

Table S5: List of distances (Å) between similar atoms present in the arms of complexed and uncomplexed [**L**.Co^{2+}] system.



x-x'	**L_1**	**CoL_1**	**$DCoL_1$-DL_1**
1-1'	5.38	5.401	-0.021
2-2'	4.687	4.519	0.168
3-3'	6.869	5.987	0.882
4-4'	6.115	4.835	1.28
5-5'	4.675	6.432	-1.757
6-6'	5.598	5.917	-0.319
7-7'	6.121	7.827	-1.706
8-8'	6.444	10.441	-3.997
9-9'	8.07	12.315	-4.245
10-10'	6.013	11.209	-5.196

Table S6. Cartesian coordinates for B3LYP/6-31G optimized structure of [**LCo]**.

Z	Coordinates			Z	Coordinates		
	x	y	z		x	y	z
1	-1.159	-4.877	-3.808	6	2.716	-2.744	2.096
1	-4.133	-3.421	-3.558	8	-0.635	-1.084	2.169
1	-2.113	-2.469	-4.124	6	0.265	-4.382	3.437
6	-0.266	-4.382	-3.437	1	-3.717	2.05	1.845
6	0.932	-5.082	-3.329	1	4.133	-3.42	3.558
6	-3.942	-3.28	-2.495	6	3.799	2.793	0.942
6	-1.684	-2.311	-3.127	6	0.35	-3.04	3.056
6	-4.922	-3.643	-1.565	1	1.159	-4.877	3.808
6	-0.35	-3.04	-3.055	1	3.292	3.755	1.002

1	-1.503	-1.237	-3.027	6	-3.799	2.794	-0.941
6	-2.716	-2.745	-2.095	6	-2.99	1.607	1.184
6	2.054	-4.451	-2.799	6	1.684	-2.311	3.127
1	2.978	-5.008	-2.667	1	3.803	2.372	1.949
6	0.813	-2.418	-2.575	7	-2.955	1.88	-0.145
6	-4.675	-3.43	-0.206	6	-1.469	-0.024	2.609
6	2.019	-3.114	-2.381	1	-0.858	0.662	3.213
1	-5.441	-3.685	0.526	1	1.503	-1.237	3.027
6	-2.439	-2.581	-0.703	6	-1.984	0.688	1.382
6	1.469	-0.024	-2.608	1	2.113	-2.47	4.124
8	0.635	-1.084	-2.168	1	-2.289	-0.381	3.238
6	-3.468	-2.891	0.237	7	-1.989	1.189	-0.76
1	4.139	-2.913	-2.262	7	-1.402	0.468	0.163
8	-1.254	-2.245	-0.28	1	-3.802	2.374	-1.948
6	3.265	-2.548	-1.709	1	0.987	-6.123	-3.636
1	5.441	-3.684	-0.526	1	5.858	-4.085	1.895
6	1.984	0.688	-1.382	1	-0.987	-6.123	3.636
7	1.402	0.468	-0.163	1	-5.858	-4.086	-1.895
6	4.675	-3.43	0.206	6	5.205	2.935	0.404
6	3.468	-2.89	-0.237	6	5.598	4.113	-0.276
1	-2.978	-5.009	2.667	6	6.127	1.881	0.621
6	-3.266	-2.548	1.709	6	6.975	4.255	-0.698
1	-4.139	-2.913	2.262	6	7.496	2.038	0.188
6	2.991	1.606	-1.184	6	5.142	6.318	-1.241
1	3.718	2.049	-1.845	6	7.388	5.448	-1.37
1	-3.298	-1.461	1.801	6	7.881	3.222	-0.447
6	4.922	-3.642	1.565	6	6.502	6.455	-1.635
6	-2.054	-4.451	2.799	1	4.439	7.115	-1.464
7	1.989	1.189	0.76	1	8.429	5.532	-1.671
6	-2.019	-3.115	2.381	1	8.915	3.339	-0.763
6	2.439	-2.581	0.703	1	6.827	7.355	-2.148
7	2.955	1.88	0.146	1	-3.291	3.757	-1
6	-0.932	-5.083	3.329	6	-5.205	2.935	-0.404
8	1.253	-2.245	0.281	6	-5.598	4.113	0.276
6	3.942	-3.279	2.495	6	-6.126	1.881	-0.621
6	-0.813	-2.418	2.576	6	-7.881	3.221	0.446
1	-8.916	3.338	0.762	6	8.039	-0.186	1.014
6	-7.495	2.037	-0.189	6	5.767	0.642	1.242
6	-8.428	0.978	-0.414	6	6.688	-0.357	1.426
6	-8.037	-0.187	-1.015	1	8.753	-0.989	1.171
6	-6.685	-0.358	-1.427	1	6.37	-1.297	1.866
1	-9.455	1.119	-0.088	1	4.743	0.459	1.549
1	-8.75	-0.99	-1.173	1	9.457	1.121	0.086
1	-6.367	-1.297	-1.867	1	3.659	5.127	-0.32
1	2.289	-0.381	-3.238	6	-6.976	4.255	0.698

1	3.297	-1.46	-1.801	6	-7.39	5.447	1.37
1	0.858	0.662	-3.212	1	-8.431	5.53	1.67
6	-5.765	0.642	-1.243	6	-6.505	6.455	1.635
6	4.708	5.194	-0.588	6	-5.144	6.318	1.241
6	8.43	0.98	0.413	6	-4.709	5.195	0.588
1	-3.66	5.128	0.321	1	-4.441	7.115	1.465
1	-4.741	0.46	-1.549	1	-6.83	7.355	2.148
27	0	-0.857	0				

Table S7. Cartesian coordinates for B3LYP/6-31G optimized structure of **L**.

Z	Coordinates			Z	Coordinates		
	x	y	z		x	y	z
8	1.42	-0.924	2.336	1	1.04	-4.659	2.757
8	1.177	0.317	-2.178	1	0.303	-3.089	2.488
8	2.547	0.902	0.107	6	4.374	-0.827	-3.627
1	2.03	0.769	-0.732	1	5.371	-0.437	-3.808
8	0.518	-1.82	-0.045	6	-4.672	-3.432	-0.577
1	0.771	-1.508	0.863	6	-1.629	0.378	-1.363
7	-2.96	0.69	-1.361	1	-1.147	-0.255	-0.636
7	-0.162	2.944	2.932	6	-1.13	0.999	-2.497
7	-0.861	2.663	4.095	6	0.539	1.849	2.51
7	-2.157	1.657	-3.141	1	1.148	1.811	1.618
7	-0.599	1.395	4.4	6	4.06	-2.142	-3.979
6	1.799	-1.866	-3.099	6	-4.337	-3.825	0.725
6	3.857	-1.064	2.507	1	-4.44	-4.87	1.005
6	2.133	-0.535	-2.798	6	0.596	-4.904	-2.002
6	2.607	-1.702	2.433	1	0.486	-5.194	-3.043
6	6.042	1.209	1.139	6	0.263	0.875	3.456
1	6.616	1.134	2.059	6	-2.247	4.299	0.845
6	2.466	-3.1	2.374	6	0.443	-2.479	-2.752
6	3.628	-3.88	2.448	1	-0.244	-1.698	-2.432
1	3.545	-4.962	2.401	1	0.023	-2.941	-3.655
6	4.883	-3.278	2.567	6	0.778	-0.515	3.598
6	3.414	-0.002	-3.025	1	1.523	-0.583	4.4
6	3.918	1.07	-0.013	1	-0.039	-1.209	3.828
6	5.933	1.635	-1.23	6	4.667	0.94	1.177
1	6.422	1.889	-2.166	6	-4.079	-1.096	0.003
6	0.777	-5.883	-1.02	6	-3.874	-2.909	1.677
6	-4.544	-2.039	-0.952	6	4.551	1.387	-1.236
6	4.993	-1.886	2.582	6	-4.019	0.368	-0.387
1	5.974	-1.422	2.634	1	-4.944	0.681	-0.876
6	3.783	1.402	-2.553	1	-3.893	1.014	0.481
1	2.883	2.018	-2.46	6	-0.837	4.386	0.985

1	4.414	1.878	-3.312	6	-0.01	4.589	-0.151
6	6.679	1.568	-0.052	6	-3.129	4.056	1.953
6	4.013	0.455	2.464	1	-2.721	3.896	2.944
1	4.641	0.766	3.308	6	-4.904	-1.676	-2.294
1	3.039	0.925	2.589	1	-4.797	-0.649	-2.621
6	0.551	-3.544	-1.67	6	0.244	1.027	-3.075
6	0.662	-3.171	-0.313	1	0.267	0.538	-4.055
6	0.88	-4.142	0.689	1	0.593	2.059	-3.197
6	0.933	-5.493	0.311	6	-5.149	-4.379	-1.539
1	1.09	-6.244	1.08	1	-5.237	-5.418	-1.237
6	-3.729	-1.51	1.315	6	0.198	4.973	-2.605
6	2.791	-2.656	-3.704	1	-0.29	5.097	-3.567
1	2.565	-3.691	-3.941	6	-3.092	-2.441	3.945
6	1.105	-3.752	2.146	1	-2.854	-2.772	4.951
6	-3.544	-3.333	3.005	1	0.774	4.732	2.392
1	-3.665	-4.384	3.251	1	-0.827	4.869	3.091
6	-4.266	4.365	-0.607	6	-4.492	3.986	1.775
1	-4.688	4.465	-1.602	1	-5.136	3.801	2.629
6	-2.844	4.451	-0.466	6	-5.073	4.144	0.482
6	-2.02	4.679	-1.575	1	-6.15	4.082	0.366
1	-2.472	4.776	-2.557	6	-3.237	-0.621	2.332
6	-0.628	4.751	-1.455	1	-3.089	0.43	2.113
6	1.426	4.634	-0.098	6	-5.36	-2.617	-3.188
1	1.938	4.48	0.844	1	-5.623	-2.316	-4.197
6	-2.933	-1.065	3.598	6	-5.486	-3.986	-2.811
1	-2.554	-0.361	4.333	1	-5.847	-4.711	-3.533
6	1.566	5.027	-2.499	6	2.184	4.847	-1.225
1	2.182	5.203	-3.375	1	3.266	4.869	-1.148
6	-0.23	4.306	2.371	7	-3.282	1.475	-2.457
1	4.808	-2.771	-4.451	1	5.776	-3.892	2.629
1	0.803	-6.933	-1.29	1	7.743	1.78	-0.063

S13. Molecular orbital (MOs) studies:

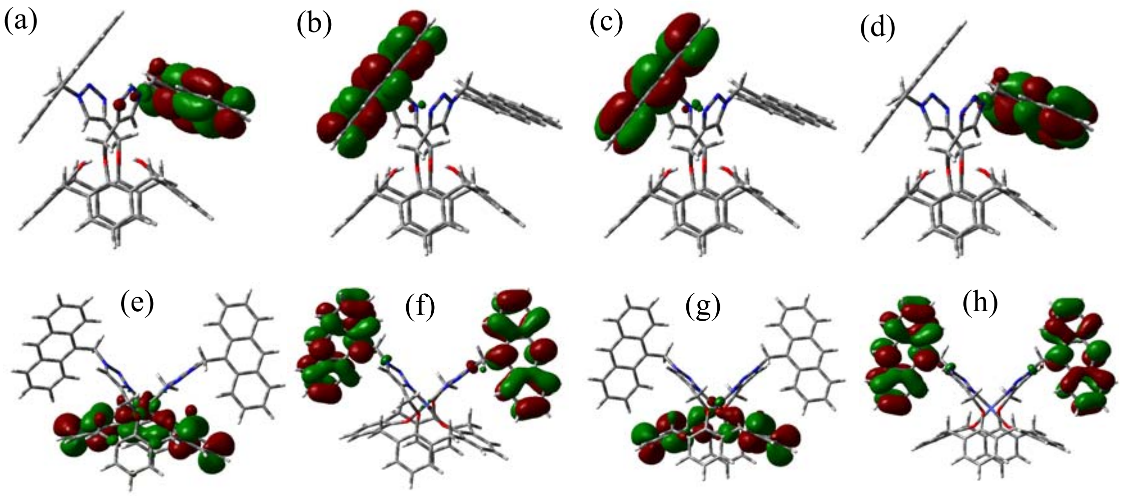


Figure S21: Molecular orbital based on DFT studies: Top row (a to d) is for **L** and bottom row (e to h) is for [Co**L**]. (a) & (e) are HOMOs; (b) & (f) are LUMOs; (c) & (g) are HOMO – 1; (d) & (h) are LUMO – 1.

S14. Molecular dynamics studies*:*

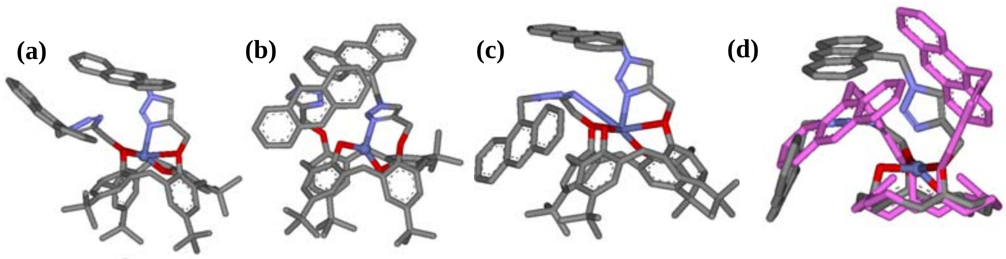


Figure S22: Conformational views of [**L**Co] structures obtained from 2 ns simulation: (a) 0.1 ns; (b) 1 ns (c) 2 ns. (d) Overlap of the structures **L** (purple, from the optimization of **L** alone) and **L** in the complex, [**L**Co] (grey).

S15. Gaussian 03 reference:

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