Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for Multifunctional Indium complexes with fluorescent sensing and selective adsorption dye properties

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Supplementary Index

1 Experimental details

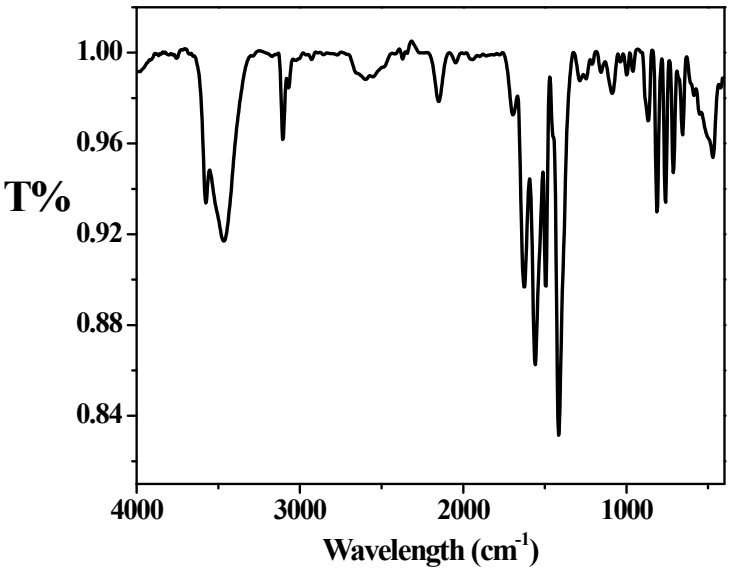
1.1 Materials

All the chemicals were analytical grade and used as purchased commercially without further purification. IR spectra were recorded on Bruker AXS TENSOR-27 FT-IR spectrometer in the KBr pellets in the range of 4000-400 cm^{-1}. Elemental analyse (C, H, and N) were performed on a Perkin-Elmer 240C automatic analyzer at the analysis center of Liaoning Normal University. UV–Vis spectra were recorded with a JASCO V-570 UV/VIS/NIR spectrophotometer in the range 200–2500 nm. The fluorescence properties of the complexes **1-4** both solid samples and in different solvent emulsions were performed on a JASCO FP-6500 spectrofluorimeter at room temperature. Powder X-ray powder diffraction (PXRD) patterns were obtained on a Bruker Advance-D8 equipped with Cu Kα radiation in the range of $5° < 2\theta < 55°$, with a step size of 0.02° (2θ) and a count time of 2 s per step.

1.2 X-ray Crystallographic Determination

X-ray diffraction data of indium complexes **1-4** were collected at room temperature on a Bruker AXS SMART APEX II CCD diffractometer with graphitemonochromated Mo-Ka radiation (λ = 0.71073). All the measured independent reflections were used for the structural analyses. A semiempirical absorption correction was adopted using program SADABS.[S1] Program SHELXTL-97 was used to check crystal-cell parameter (XPREP), crystal structure was solved by the direct method (XS) and least-squares refinement (XL).[S2] Hydrogen atoms of coordination water molecules and lattice water molecules were found in the difference Fourier map. The positions of indium atom, oxygen atom, carbon atom and nitrogen atom were determined at first, all hydrogen atoms were fixed at calculated positions with isotropic thermal parameters except for the coordinated water molecules.

2 IR spectra



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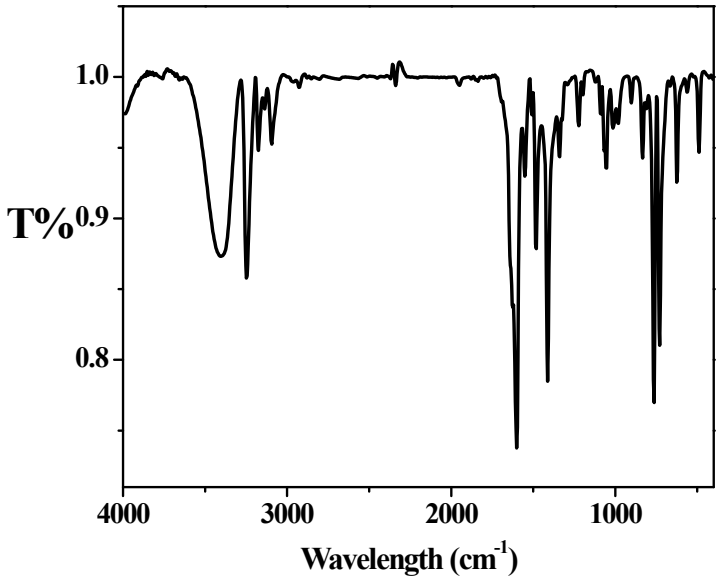

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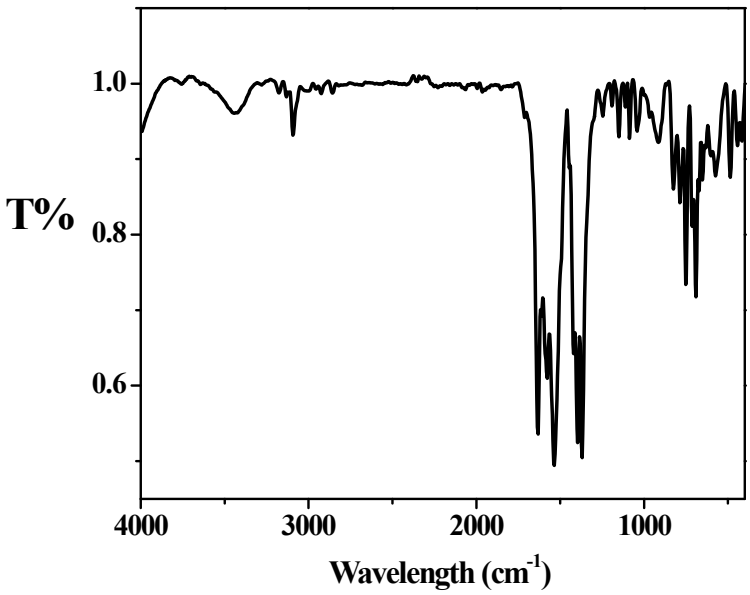

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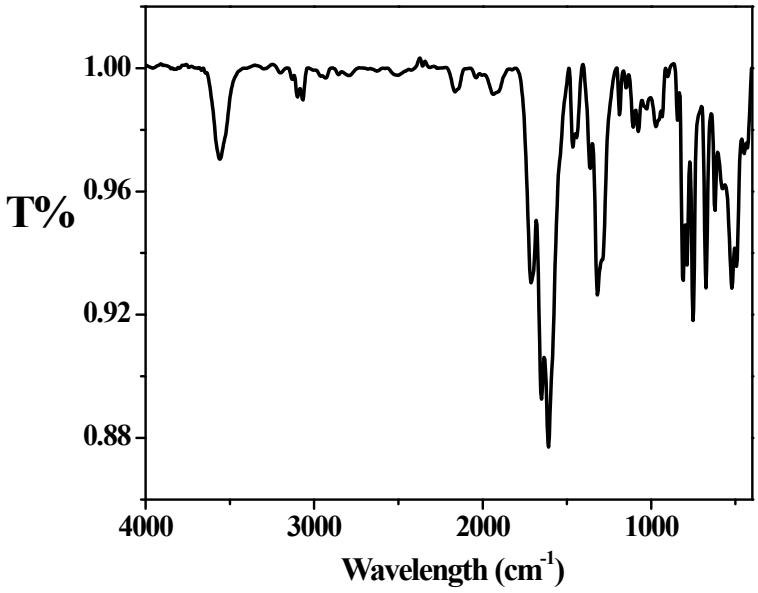
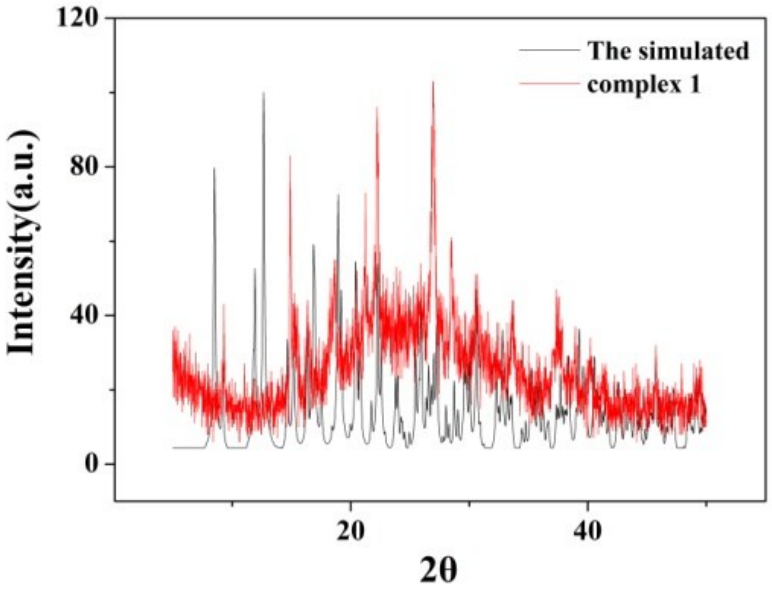


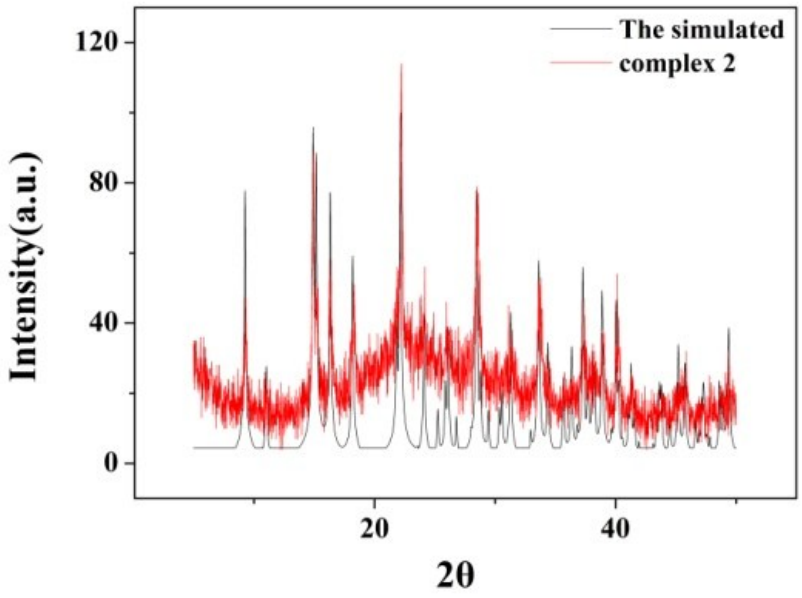
(**4**)

Fig. S1 The IR spectra of complexes **1–4**

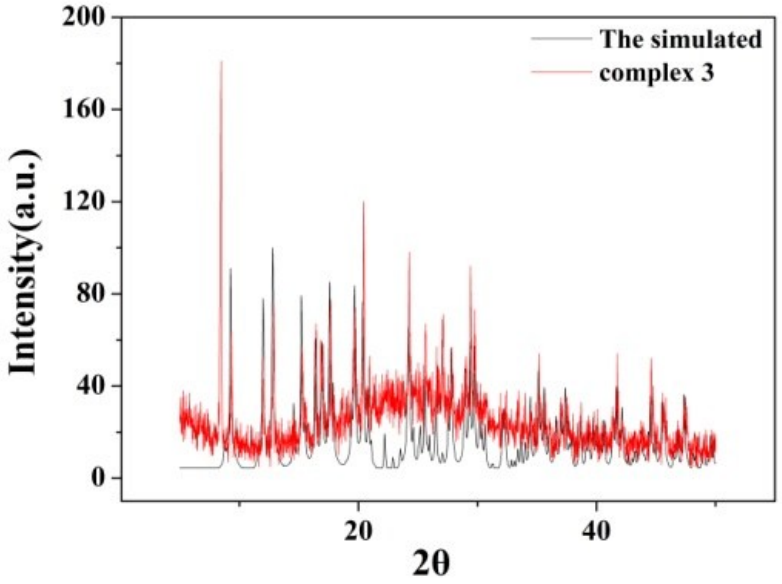
3 PXRD


120
80
40
0
Intensity(a.u.)
20
40
2θ
The simulated
complex 1

(**1**)


120
80
40
0
Intensity(a.u.)
20
40
2θ
The simulated
complex 2

(**2**)



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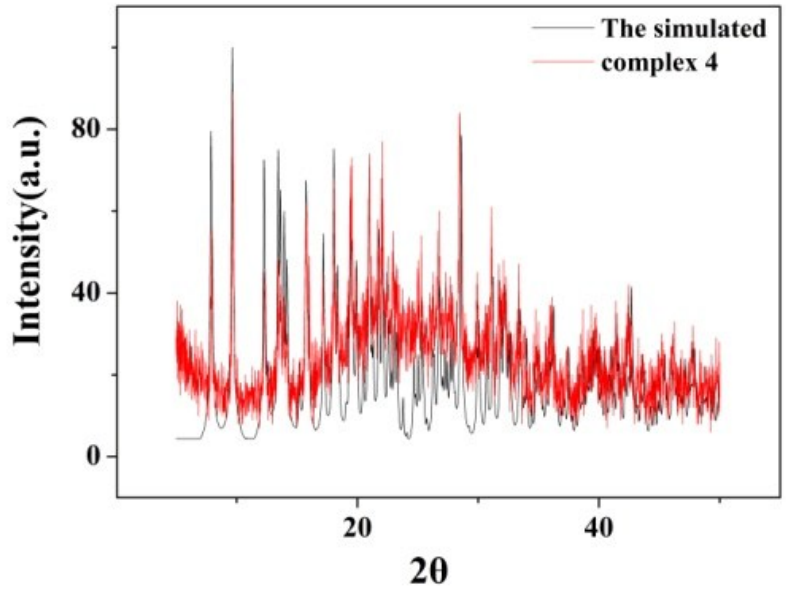
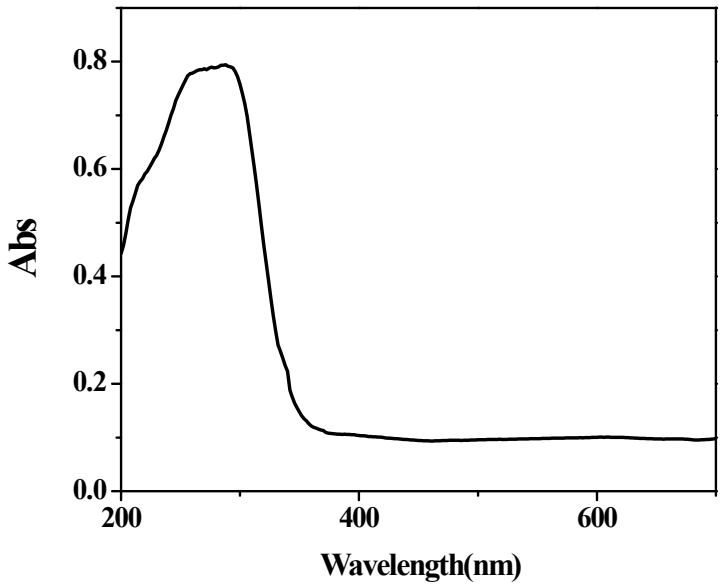


(**4**)

Fig. S2 The PXRD pattern based on the X-ray single crystal diffraction of the complexes **1-4**, and the experimental samples of the complexes **1-4**, respectively

4 UV-Vis spectra



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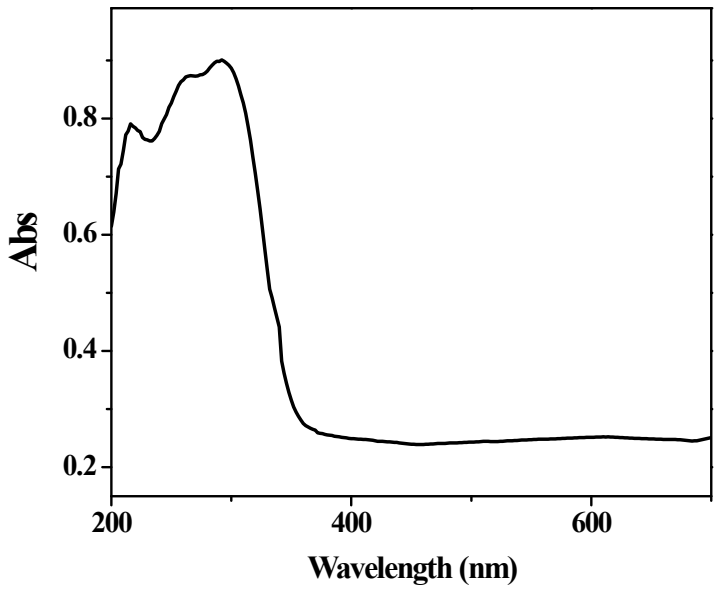

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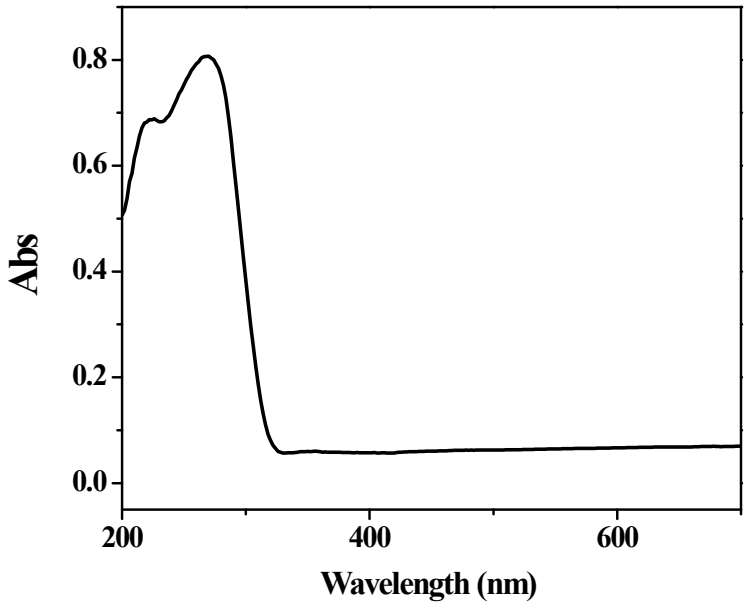

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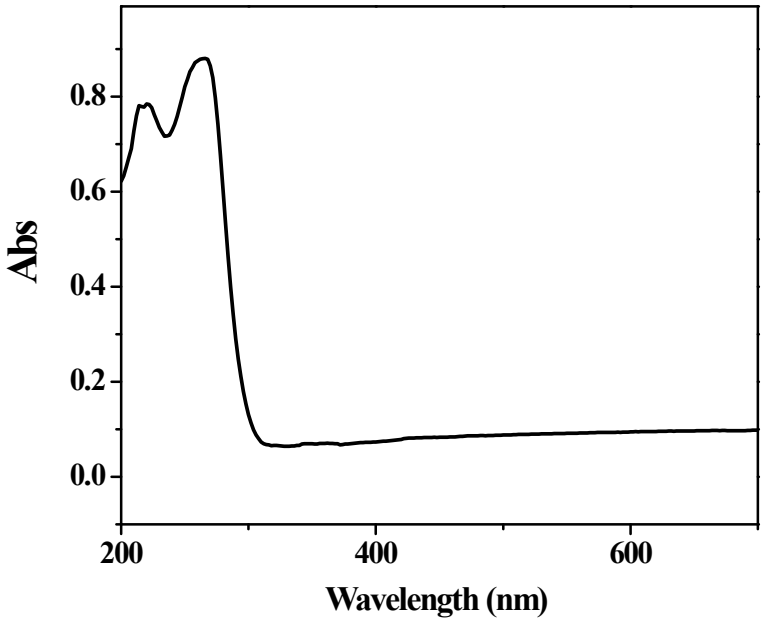
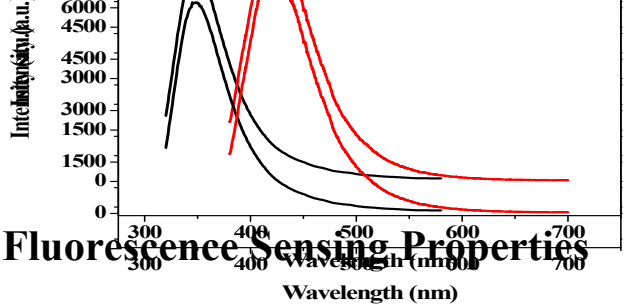
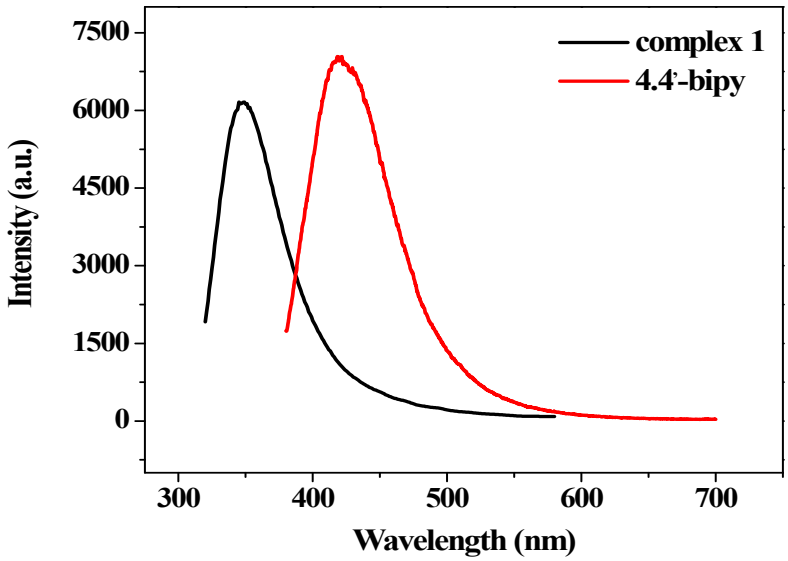


(**4**)

Fig. S3 The IR spectra of complexes **1-4**



5 Fluorescence Sensing Properties



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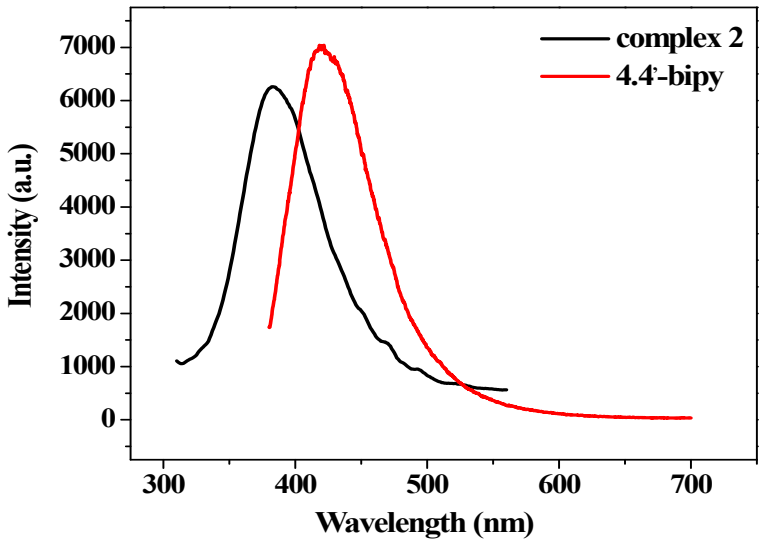

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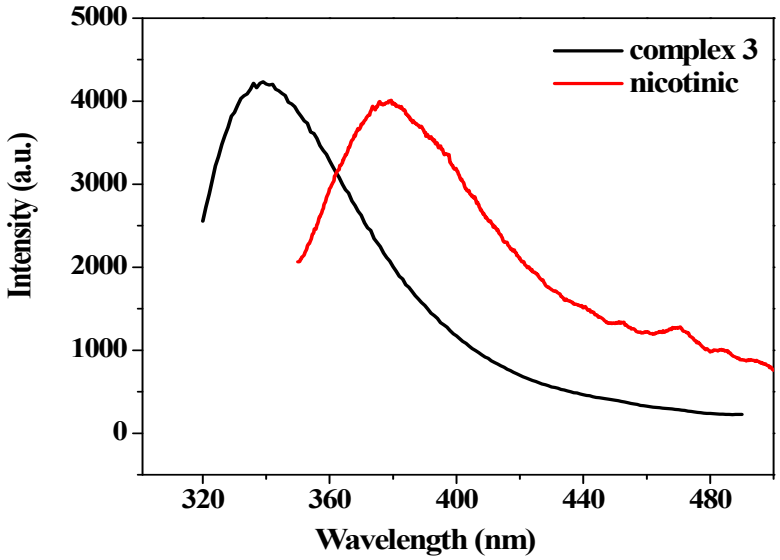

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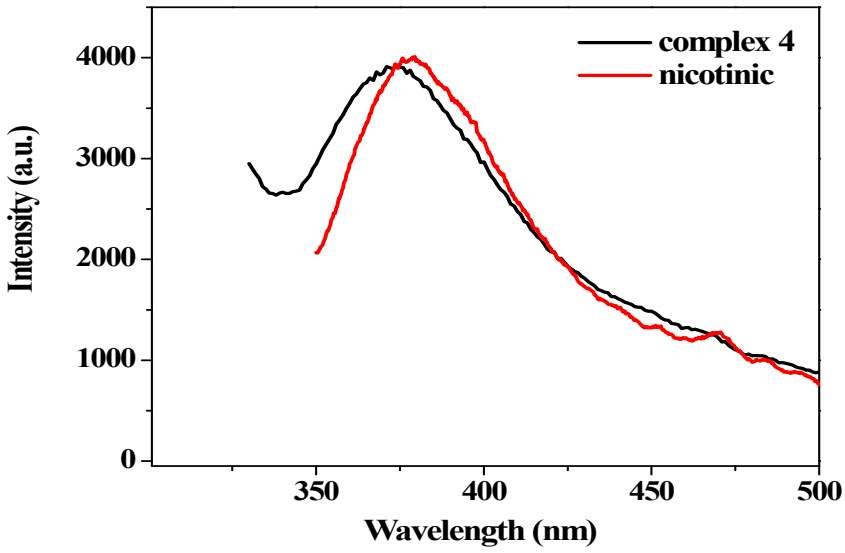

(4)

Fig. S4 Fluorescence spectra of the ligand and **1-4** in the solid state.

6 Crystal data

Table S1 Selected bond distances (Å) and angles (°) of the complexes **1**-**4**

Complex **1**			
In(1)-O(1)	2.323(2)	In(1)-O(2)	2.300(2)
In(1)-O(3)	2.208(2)	In(1)-O(4)#1	2.215(2)
In(1)-O(5)#1	2.438(16)	In(1)-Cl(1)	2.4216(9)
In(1)-Cl(2)	2.4539(9)	O(4)-In(1)#3	2.215(2)
O(5)-In(1)#3	2.438(16)		
O(1)-In(1)-O(5)#1	168.5(3)	O(1)-In(1)-Cl(1)	92.67(6)
O(1)-In(1)-Cl(2)	85.65(6)	O(2)-In(1)-O(1)	56.30(8)
O(2)-In(1)-O(5)#1	133.1(3)	O(2)-In(1)-Cl(1)	92.95(7)
O(2)-In(1)-Cl(2)	141.19(6)	O(3)-In(1)-O(1)	86.12(8)
O(3)-In(1)-O(2)	84.24(9)	O(3)-In(1)-O(4)#1	81.63(9)
O(3)-In(1)-O(5)#1	88.4(4)	O(3)-In(1)-Cl(1)	177.16(7)
O(3)-In(1)-Cl(2)	86.01(7)	O(4)#1-In(1)-O(1)	134.90(8)
O(4)#1-In(1)-O(2)	79.29(8)	O(4)#1-In(1)-O(5)#1	53.8(3)
O(4)#1-In(1)-Cl(1)	97.46(7)	O(4)#1-In(1)-Cl(2)	135.97(7)
O(5)#1-In(1)-Cl(2)	83.9(3)	Cl(1)-In(1)-O(5)#1	93.2(4)
Cl(1)-In(1)-Cl(2)	96.47(3)		
Complex **2**			
In(1)-O(1)	2.210(5)	In(1)-N(1)	2.330(6)
In(1)-Cl(1)#1	2.4777(14)	In(1)-Cl(1)#2	2.4777(14)
In(1)-Cl(1)	2.4777(14)	In(1)-Cl(1)#3	2.4777(14)
O(1)-In(1)-N(1)	180.000(1)	O(1)-In(1)-Cl(1)#1	89.53(3)
N(1)-In(1)-Cl(1)#1	90.47(3)	O(1)-In(1)-Cl(1)#2	89.53(3)
N(1)-In(1)-Cl(1)#2	90.47(3)	Cl(1)#1-In(1)-Cl(1)#2	91.11(7)
O(1)-In(1)-Cl(1)	89.53(3)	N(1)-In(1)-Cl(1)	90.47(3)
Cl(1)#1-In(1)-Cl(1)	88.88(7)	Cl(1)#2-In(1)-Cl(1)	179.06(6)
O(1)-In(1)-Cl(1)#3	89.53(3)	N(1)-In(1)-Cl(1)#3	90.47(3)
Cl(1)#1-In(1)-Cl(1)#3	179.06(6)	Cl(1)#2-In(1)-Cl(1)#3	88.88(7)
Cl(1)-In(1)-Cl(1)#3	91.11(7)	In(1)-O(1)-H(1A)	121(5)
Complex **3**			
In(1)-Cl	2.412(3)	In(1)-O(1)	2.173(6)
In(1)-O(4)	2.144(7)	In(1)-O(6)#1	2.103(6)
In(1)-O(7)	2.168(7)	In(1)-O(8	2.204(7)
O(1)-In(1)-Cl	93.6(3)	O(1)-In(1)-O(8)	83.8(3)
O(4)-In(1)-Cl	175.1(2)	O(4)-In(1)-O(1)	88.1(4)
O(4)-In(1)-O(7)	81.6(3)	O(4)-In(1)-O(8)	90.7(3)
O(6)#1-In(1)-Cl	91.3(3)	O(6)#1-In(1)-O(1)	168.6(3)
O(6)#1-In(1)-O(4)	87.9(4)	O(6)#1-In(1)-O(7)	103.7(3)
O(6)#1-In(1)-O(8)	85.6(4)	O(7)-In(1)-Cl	93.9(2)
O(7)-In(1)-O(1)	86.2(3)	O(7)-In(1)-O(8)	167.6(3)
O(8)-In(1)-Cl	94.1(2)	C(6)-O(1)-In(1)	132.8(8)

C(7)-O(4)-In(1)	131.3(7)	C(14)-O(6)-In(1)#2	127.7(8)
In(1)-O(7)-H(7A)	111.6	In(1)-O(7)-H(7B)	110.7
Complex **4**			
In(1)-Cl(1)	2.3791(7)	In(1)-O(1)	2.2289(14)
In(1)-O(2)	2.2166(13)	In(1)-O(5)	2.1524(13)
In(1)-O(6)#1	2.2186(14)	In(1)-O(8)#2	2.2459(13)
O(6)-In(1)#1	2.2186(14)	O(8)-In(1)#	2.2459(13)
O(1)-In(1)-Cl(1)	101.38(5)	O(1)-In(1)-O(7)	142.45(5)
O(1)-In(1)-O(8)#2	142.62(5)	O(2)-In(1)-Cl(1)	91.08(5)
O(2)-In(1)-O(1)	72.61(5)	O(2)-In(1)-O(6)#1	144.02(5)
O(2)-In(1)-O(7)	144.81(5)	O(2)-In(1)-O(8)#2	75.40(5)
O(5)-In(1)-Cl(1)	170.30(4)	O(5)-In(1)-O(1)	88.04(5)
O(5)-In(1)-O(2)	93.95(6)	O(5)-In(1)-O(6)#1	87.78(6)
O(5)-In(1)-O(7)	86.32(6)	O(5)-In(1)-O(8)#2	75.30(5)
O(6)#1-In(1)-Cl(1)	93.01(5)	O(6)#1-In(1)-O(1)	71.53(5)
O(6)#1-In(1)-O(7)	71.17(5)	O(6)#1-In(1)-O(8)#2	138.95(5)
O(7)-In(1)-Cl(1)	84.79(5)	O(8)#2-In(1)-Cl(1)	98.03(4)
O(8)#2-In(1)-O(7)	70.65(5)	C(4)-O(1)-In(1)	117.05(11)
C(3)-O(2)-In(1)	117.87(11)	C(1)-O(5)-In(1)	116.13(11)
C(2)-O(6)-In(1)#1	118.61(12)	C(2)-O(7)-In(1)	115.15(11)
C(1)-O(8)-In(1)#2	113.28(10)		

Symmetry transformations used to generate equivalent atoms: complex **1**: #1 x, -y+3/2, z+1/2; #2 -x+1, -y+2, -z+2; #3 x, -y+3/2, z-1/2; complex **2**: #1 -x+1, y, z; #2 -x+1, y, -z+1/2; #3 x, y, -z+1/2; complex **3**: #1 x-1/2, -y+1/2, -z; #2 x+1/2, -y+1/2, -z; complex **4**: #1 -x, -y+1, -z+2; #2 -x+1, -y+1, -z+2;

Table S2 Hydrogen bond lengths (Å) and angles (°) for the complexes **1**-**4**

Complex **1**				
D–H···A	D–H	H···A	D···A	D–H···A
C(10)-H(10)...Cl(2)#5	0.93	2.85	3.758(4)	164.7
C(13)-H(13)...O(2W)	0.93	2.57	3.302(6)	136.0
O(1W)-H(1WA)...O(2W)#3	0.85	2.51	3.130(5)	130.9
O(1W)-H(1WB)...O(5)	0.85	2.54	3.189(14)	133.5
O(1W)-H(1WB)...Cl(2)#3	0.85	2.54	3.278(3)	146.3
O(2W)-H(2WA)...Cl(1)#7	0.85	2.67	3.360(3)	139.6
O(2W)-H(2WA)...Cl(2)#1	0.85	2.79	3.314(3)	121.9
O(3)-H(3A)...Cl(2)#1	0.88	2.95	3.487(2)	120.7
Complex **2**				
D–H···A	D–H	H···A	D···A	D–H···A
O(1)-H(1A)...Cl(1)#4	0.815(10)	2.80(2)	3.387(4)	130(3)
O(1)-H(1A)...Cl(1)#5	0.815(10)	2.80(2)	3.387(4)	130(3)
N(2)-H(2A)...Cl(1)#6	0.858(10)	2.973(6)	3.477(5)	119.5(2)
N(2)-H(2A)...Cl(1)#7	0.858(10)	2.973(6)	3.477(5)	119.5(2)
N(2)-H(2A)...Cl(1)#8	0.858(10)	2.973(6)	3.477(5)	119.5(2)
N(2)-H(2A)...Cl(1)#9	0.858(10)	2.973(6)	3.477(5)	119.5(2)

Complex **3**				
D–H···A	D–H	H···A	D···A	D–H···A
N(1)-H(1)...O(7)#4	0.86	2.55	3.169(12)	129.6
C(3)-H(3)...Cl#6	0.93	2.98	3.630(15)	128.3
Complex **4**				
D–H···A	D–H	H···A	D···A	D–H···A
C(5)-H(5)...Cl(1)#7	0.93	2.64	3.508(2)	156.6
C(7)-H(7)...O(11)	0.93	2.65	3.467(3)	146.4
C(13)-H(13)...O(6)#2	0.93	2.50	3.293(3)	143.3
C(13)-H(13)...O(7)#2	0.93	2.62	3.368(3)	138.3

*Symmetry transformation used to generate equivalent atoms: complex **1**: #1 x, -y+3/2, z+1/2; #3 x, -y+3/2, z-1/2; #5 -x+1, y+1/2, -z+3/2; #7 x+1, -y+3/2, z+1/2; complex **2**: #4 -x+1, -y+2, z+1/2; #5 -x+1, -y+2, -z; #6 -x+1, -y+1, -z; #7 x, -y+1, z+1/2; #8 x, -y+1, -z; #9 -x+1, -y+1, z+1/2; complex **3**: #4 -x+1, y+1/2, -z+1/2; #6 -x+1/2, -y+1, z+1/2; complex **4**: #2 -x+1, -y+1, -z+2; #7 x, y+1, z;

7 References

S1 G. M. Sheldrick*, SADABS,* Program for Empirical Absorption Correction for area Detector Data; University of Gottingen, Gottingen, Germany, 1996.

S2 G. M. Sheldrick*, SHELXS 97*, Program for Crystal Structure Refinement;