Electronic Supplementary Information for Dalton Transactions

Supplementary material (ESI):

Synthesis, Crystal structure and Optical properties of $[Ag(UO_2)_3(OAc)_9][Zn(H_2O)_4(CH_3CH_2OH)_2]$: A Novel Compound Containing Closed-shell $3d^{10}$, $4d^{10}$ and $5d^{10}$ Metal Ions

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Electronic Supporting Information

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1. Experimental Procedures

IR spectra were s recorded on a Nicolet AVATAT FT-IR360 spectrometer as KBr pellets in the frequency range 4000-400 cm^{-1}. ^{1}H NMR and ^{13}C NMR were acquired in $CDCl_3$ on Varian Unity^{+} 400MHz NMR spectrometer using TMS as an internal standard. Powder X-ray diffraction (PXRD) data were collected on a Philips X'Pert Pro MPD X-ray diffractometer with Cu K_{α} radiation equipped with a X'Celerator detector. The elemental analyses (C, H, N contents) were determined on a CE instruments EA 1110 analyzer. The emission of dark-green light from **1** is easily observed when the sample is irradiated with 254 or 356 nm UV light using a handheld UV lamp. Photoluminescence measurements were performed on a Hitachi F-4500 fluorescence spectrophotometer with solid powder on a 1 cm quartz round plate (for emission spectra, excitation wavelength: 365, 424 and 447 nm; emission wavelengths: 400-800 nm; slit width: 2.5 nm; sensitivity: high. for excitation spectra, emission wavelength: 481, 501, 523 and 546 nm; excitation wavelengths: 300-500 nm; slit width: 2.5 nm; sensitivity: high).

2. Tables of anisotropic thermal parameters, selected bond distances and angles and hydrogen bond geometry for **1.**

Table S1. atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn1	2500	7500	0000	29(1)
Ag1	5000	2508(1)	2500	43(1)
U1	5000	5406(1)	2500	36(1)
U2	6470(2)	846(1)	2541(3)	33(1)
C1	7490(6)	-313(8)	2587(9)	36(3)
C2	8052(8)	-886(1)	2635(15)	80(6)
C3	6122(6)	746(9)	3986(9)	40(3)
C4	5910(8)	685(12)	4704(12)	70(5)

C5	5770(6)	2185(9)	1048(9)	46(3)
C6	5430(8)	2904(12)	312(13)	79(5)
C7	6134(6)	4351(10)	3853(10)	50(3)
C8	6706(8)	3817(11)	4569(12)	76(5)
C9	5000	7429(12)	2500	43(5)
C10	5000	8509(13)	2500	67(6)
C11	3104(7)	7071(10)	2173(10)	56(4)
C12	3584(8)	7387(13)	3135(10)	69(5)
O1	5856(4)	-3(6)	1904(7)	50(2)
O2	7078(4)	1713(6)	3176(6)	48(2)
O3	5881(5)	1348(6)	3343(8)	59(3)
O4	6552(4)	185(6)	4007(6)	45(2)
O5	7368(4)	-341(6)	3245(6)	45(2)
O6	7120(4)	204(6)	1862(7)	49(2)
O7	6226(4)	1654(6)	1069(6)	48(2)
O8	5645(4)	2093(6)	1693(7)	52(2)
O9	6149(4)	5247(6)	3869(7)	55(2)
O10	5619(4)	3951(6)	3240(8)	58(3)
O11	4691(4)	5411(6)	3280(7)	58(3)
O12	5517(4)	6986(6)	3060(6)	44(2)
O13	3197(4)	7476(6)	1464(6)	39(2)
O1W	3134(4)	8508(6)	-39(6)	48(2)
O2W	1975(4)	8531(5)	260(6)	39(2)

Table S2 Selected bond lengths (Å) and angles (°) for **1**

Ag(1)-O(3)	2.412(9)	Ag(1)-O(3)^{ii}	2.412(9)	Ag(1)-O(10)	2.414(9)
Ag(1)-O(10)^{ii}	2.414(9)	Ag(1)-O(8)	2.483(8)	Ag(1)-O(8)^{ii}	2.483(8)
U(1)-O(11)	1.732(9)	U(1)-O(11)^{ii}	1.732(9)	U(1)-O(10)	2.427(8)
U(1)-O(10)^{ii}	2.427(8)	U(1)-O(12)	2.455(8)	U(1)-O(12)^{ii}	2.455(8)
U(1)-O(9)	2.467(8)	U(1)-O(9)^{ii}	2.467(8)	U(2)-O(1)	1.734(9)
U(2)-O(2)	1.743(8)	U(2)-O(3)	2.402(8)	U(2)-O(6)	2.423(8)
U(2)-O(8)	2.432(8)	U(2)-O(5)	2.439(7)	U(2)-O(7)	2.440(8)
U(2)-O(4)	2.473(8)	Zn(1)-O(13)	2.101(8)	Zn(1)-O(13)^{i}	2.101(8)
Zn(1)-O(1w)	2.047(7)	Zn(1)-O(1w)^{i}	2.047(7)	Zn(1)-O(2w)	2.051(7)
Zn(1)-O(2w)^{i}	2.051(7)				

O(3)-Ag(1)-O(3)^{ii}	95.6(5)	O(10)-Ag(1)-O(3)^{ii}	164.1(3)
O(3)-Ag(1)-O(10)	99.3(3)	O(3)-Ag(1)-O(10)^{ii}	164.1(3)
O(10)-Ag(1)-O(10)^{ii}	66.6(4)	O(3)^{ii} -Ag(1)-O(8)	95.4(3)
O(3)-Ag(1)-O(8)	66.0(3)	O(10)-Ag(1)-O(8)	95.8(3)
O(10)^{ii} -Ag(1)-O(8)	106.8(3)	O(3)^{ii}-Ag(1)-O(8)^{ii}	66.0(3)

O(3)-Ag(1)-O(8)^{ii}	95.4(3)	O(10)^{ii}-Ag(1)-O(8)	106.8(3)
O(10)^{ii}-Ag(1)-O(8)^{ii}	95.8(3)	O(10)-Ag(1)-O(8)^{ii}	106.8(3)
O(10)^{ii}-Ag(1)-O(8)^{ii}	95.7(3)	O(8)-Ag(1)-O(8)^{ii}	153.0(4)
O(11)^{ii}-U(1)-O(11)	179.5(6)	O(11)^{ii}-U(1)-O(10)^{ii}	89.6(4)
O(11)-U(1)-O(10)^{ii}	90.8(4)	O(11)^{ii}-U(1)-O(10)	90.8(4)
O(11)-U(1)-O(10)	89.6(4)	O(10)^{ii}-U(1)-O(10)	66.2(4)
O(11)^{ii}-U(1)-O(12)	88.2(4)	O(11)-U(1)-O(12)	91.3(4)
O(10)^{ii}-U(1)-O(12)	172.5(3)	O(10)-U(1)-O(12)	121.0(3)
O(11)^{ii}-U(1)-O(12)^{ii}	91.3(4)	O(11)-U(1)-O(12)^{ii}	88.3(4)
O(10)^{ii} -U(1)-O(12)^{ii}	121.0(3)	O(10)-U(1)-O(12)^{ii}	172.5(3)
O(12)-U(1)-O(12)^{ii}	51.9(4)	O(11)^{ii}-U(1)-O(9)^{ii}	89.1(4)
O(11)-U(1)-O(9)^{ii}	91.0(4)	O(10)^{ii} -U(1)-O(9)^{ii}	51.7(3)
O(10)-U(1)-O(9)^{ii}	117.9(3)	O(12)-U(1)-O(9)^{ii}	121.0(3)
O(12)^{ii} -U(1)-O(9)^{ii}	69.3(3)	O(11)^{ii} -U(1)-O(9)	91.0(4)
O(11)-U(1)-O(9)	89.1(4)	O(10)^{ii}-U(1)-O(9)	117.9(3)
O(10)-U(1)-O(9)	51.7(3)	O(12)-U(1)-O(9)	69.3(3)
O(12)^{ii}-U(1)-O(9)	121.0(3)	O(9)^{ii}-U(1)-O(9)	169.7(4)
O(1)-U(2)-O(2)	179.1(4)	O(1)-U(2)-O(3)	90.8(4)
O(2)-U(2)-O(3)	88.6(4)	O(1)-U(2)-O(6)	88.6(3)
O(2)-U(2)-O(6)	92.0(3)	O(3)-U(2)-O(6)	173.7(3)
O(1)-U(2)-O(8)	89.0(4)	O(2)-U(2)-O(8)	90.2(4)
O(3)-U(2)-O(8)	67.0(3)	O(6)-U(2)-O(8)	119.3(3)
O(1)-U(2)-O(5)	93.4(4)	O(2)-U(2)-O(5)	87.5(3)
O(3)-U(2)-O(5)	121.0(3)	O(6)-U(2)-O(5)	52.8(3)
O(8)-U(2)-O(5)	171.6(3)	O(1)-U(2)-O(7)	90.6(4)
O(2)-U(2)-O(7)	89.0(4)	O(3)-U(2)-O(7)	118.6(3)
O(6)-U(2)-O(7)	67.6(3)	O(8)-U(2)-O(7)	51.7(3)
O(5)-U(2)-O(7)	120.1(3)	O(1)-U(2)-O(4)	88.1(4)
O(2)-U(2)-O(4)	92.0(4)	O(3)-U(2)-O(4)	51.6(3)
O(6)-U(2)-O(4)	122.1(3)	O(8)-U(2)-O(4)	118.5(3)
O(5)-U(2)-O(4)	69.7(3)	O(7)-U(2)-O(4)	170.1(3)
U(2)-O(8)-Ag(1)	111.6(3)	Ag(1)-O(10)-U(1)	113.6(4)
C(11)-O(13)-Zn(1)	126.7(7)	O(1w)-Zn(1)-O(1w)^{i}	180.000(1)
O(1w)^{i}-Zn(1)-O(2w)	88.8(3)	O(1w)^{i}-Zn(1)-O(2w)^{i}	91.2(3)
O(1w)-Zn(1)-O(2w)	91.2(3)	O(1w) -Zn(1)-O(2w)^{i}	88.8(3)
O(2w) ^{i}-Zn(1)-O(2w)	180.0(5)	O(1w)-Zn(1)-O(13)^{i}	96.0(3)
O(1w)^{i} -Zn(1)-O(13)^{i}	83.6(3)	O(2w)^{i} -Zn(1)-O(13)^{i}	88.4(3)
O(2w)-Zn(1)-O(13)^{i}	91.6(3)	O(1w)-Zn(1)-O(13)	84.0(3)
O(1w) ^{i}-Zn(1)-O(13)	96.0(3)	O(2w) ^{i}-Zn(1)-O(13)	91.6(3)
O(2w)-Zn(1)-O(13)	88.4(3)	O(13) ^{i}-Zn(1)-O(13)	180.0(4)

[a] Symmetry code i，-x+1/2, -y+3/2, -z; ii, -x+1, y, -z+1/2

Table S3 Hydrogen bond geometry (Å, °) for **1**

D-H…A	D-H	H···A	D···A	D-H···A
O(13)-H(13B)…O(12) [i]	0.82	1.96	2.733(10)	158.1
O(1w)-H(1wA)…O(4) [ii]	0.82	2.36	2.759(11)	110.4
O(1w)-H(1wB)…O(7) [iii]	0.82	1.95	2.728(10)	158.8
O(2w)-H(2wD)…O(9) □	0.82	2.08	2.708(11)	132.9
O(2w)-H(2wA)…O(5) [ii]	0.82	1.94	2.645(11)	143.0

Symmetry codes: (i), -x+1, y, -z +1/2; (ii), -x+1, y+1, -z+1/2; (iii), -x+1, -y+1, -z; (iv), x-1/2, -y+3/2, z-1/2

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **1**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zn(1)	32(1)	25(1)	26(1)	0(1)	11(1)	0(1)
Ag(1)	39(1)	25(1)	60(1)	0	23(1)	0
U(1)	31(1)	25(1)	37(1)	0	6(1)	0
U(2)	36(1)	30(1)	31(1)	8(1)	16(1)	4(1)
C(1)	41(7)	35(7)	35(7)	6(6)	22(6)	-2(5)
C(2)	83(12)	76(11)	115(17)	12(11)	76(14)	24(9)
C(3)	50(8)	45(7)	31(7)	16(6)	26(6)	20(6)
C(4)	82(11)	82(11)	62(11)	36(9)	51(10)	34(9)
C(5)	43(8)	55(8)	30(7)	18(7)	10(6)	0(6)
C(6)	72(11)	78(11)	86(14)	36(11)	39(11)	13(9)
C(7)	32(7)	48(8)	42(8)	6(7)	-1(6)	-3(6)
C(8)	72(11)	57(9)	53(10)	15(8)	-4(8)	26(8)
C(9)	42(12)	33(9)	61(14)	0	29(11)	0
C(10)	78(16)	25(10)	83(18)	0	26(14)	0
C(11)	54(9)	63(9)	51(9)	10(8)	25(8)	-21(7)
C(12)	63(10)	115(14)	18(7)	7(8)	8(7)	6(9)
O(1)	46(5)	50(5)	49(6)	15(5)	19(5)	-2(4)
O(1W)	58(6)	41(5)	44(6)	-15(4)	28(5)	-19(4)
O(2W)	42(5)	31(4)	34(5)	0(4)	14(4)	10(3)
O(2)	45(5)	44(5)	39(5)	7(4)	9(4)	-2(4)
O(3)	73(7)	50(6)	68(7)	24(5)	45(6)	34(5)
O(4)	56(5)	44(5)	43(5)	19(4)	31(5)	17(4)
O(5)	53(5)	40(5)	39(5)	20(4)	20(5)	26(4)

O(6)	57(6)	50(5)	39(6)	-6(5)	23(5)	-8(4)
O(7)	56(6)	61(6)	34(5)	21(5)	28(5)	14(5)
O(8)	53(6)	61(6)	45(6)	24(5)	30(5)	27(5)
O(9)	43(5)	31(5)	46(6)	0(4)	-14(4)	-5(4)
O(10)	41(5)	31(5)	66(7)	2(4)	0(5)	5(4)
O(11)	52(6)	55(6)	58(7)	12(5)	21(5)	0(5)
O(12)	26(4)	39(5)	50(6)	-5(4)	6(4)	-4(4)
O(13)	31(5)	53(5)	26(5)	12(4)	8(4)	1(4)

3. Figure S1 and S2: Polyhedral representation and Schematic depiction of crystal packing of **1**.

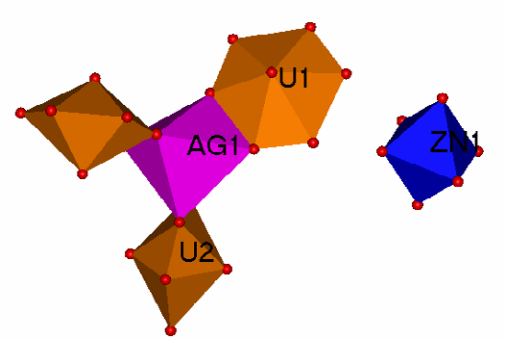

Figure S1 Polyhedral representation showing only the atoms coordinated directly to U, Ag and Zn for clarity.

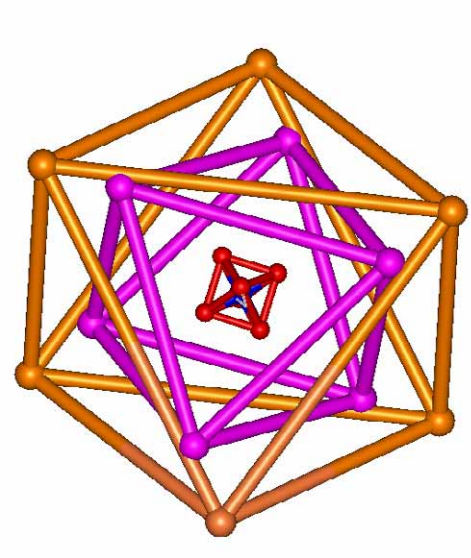

Figure S2 Schematic depiction of crystal packing of **1**.

4. IR spectra of compound **1**(Figure S3)

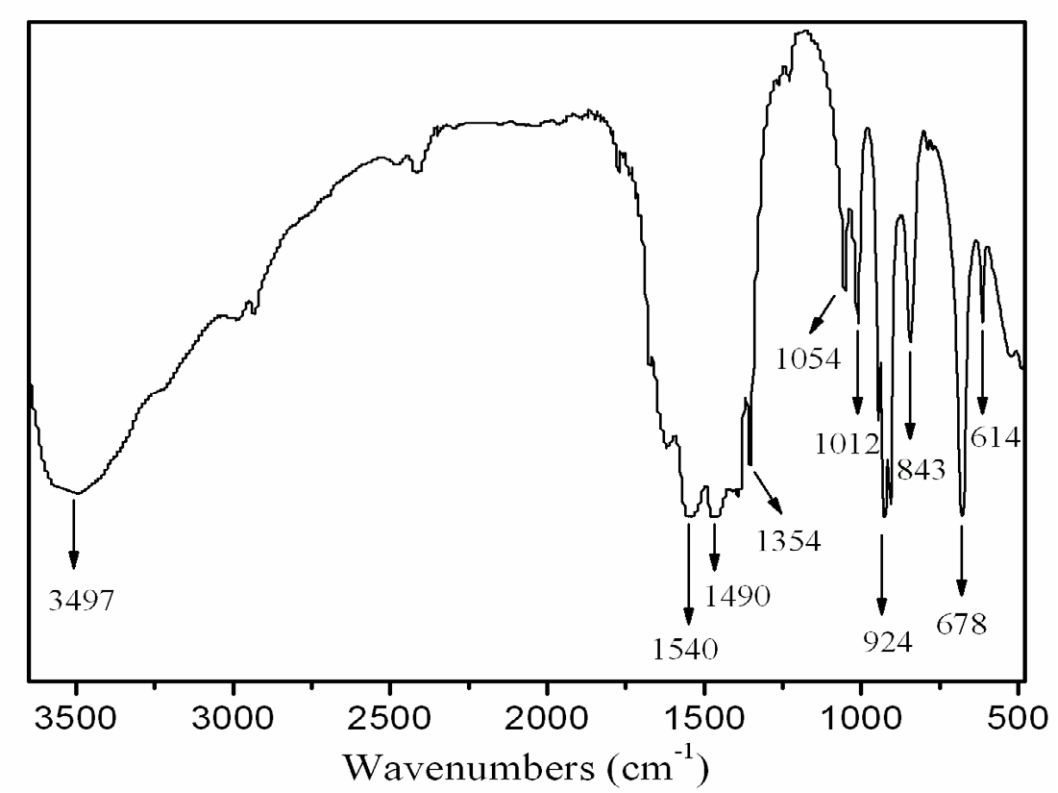

Figure S3: IR spectra of **1**. Note that the peaks at 3497, 1540, 1459 and 924 cm^{-1}, ascribed to ν(OH), ν_{as}(COO), ν_s(COO) and $\nu(UO_2^{2+})$ stretching absorptions of **1** respectively.

5. ^{1}H NMR and ^{13}C NMR of **1**(Figure S4 & S5)

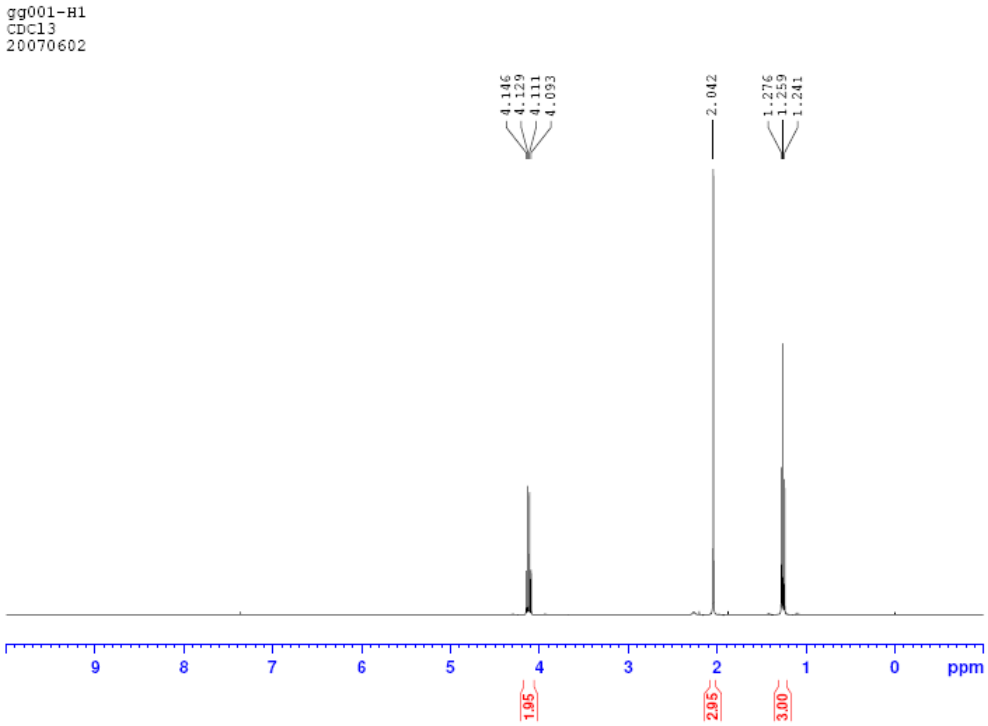

Figure S4: ^{1}H NMR of **1**. δ (ppm) = 4.13 (2H, m), 2.04(1H, s), 1.26(3H, t), respectively.

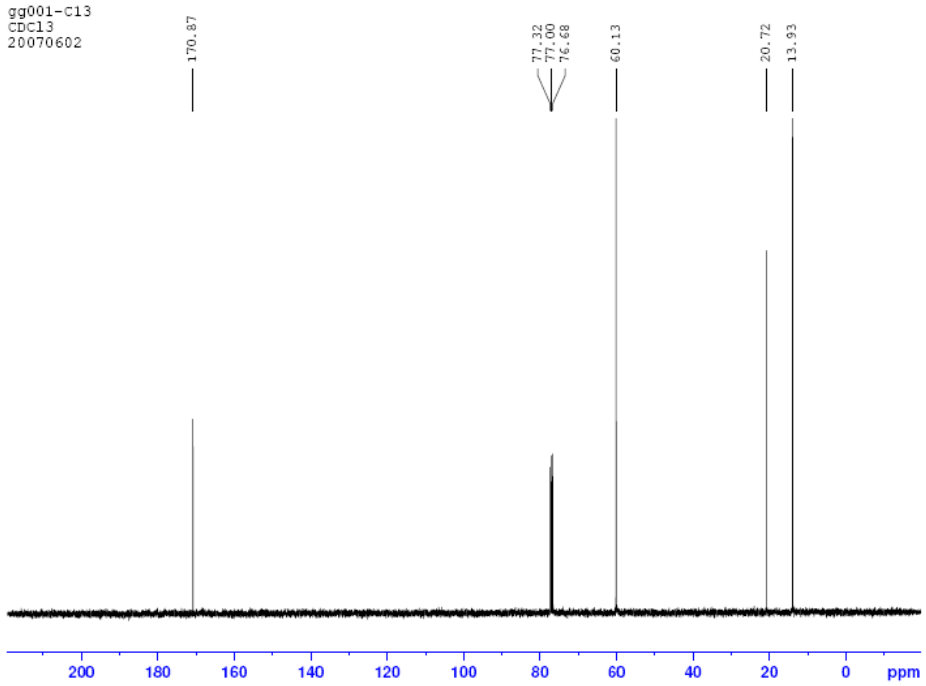

Figure S5: ^{13}C NMR of **1**. δ (ppm) = 13.93, 20.72, 60.13, 76.68, 77.00, 77.32, 170.87.

5. Powder XRD patterns of compound **1**(Figure S6)

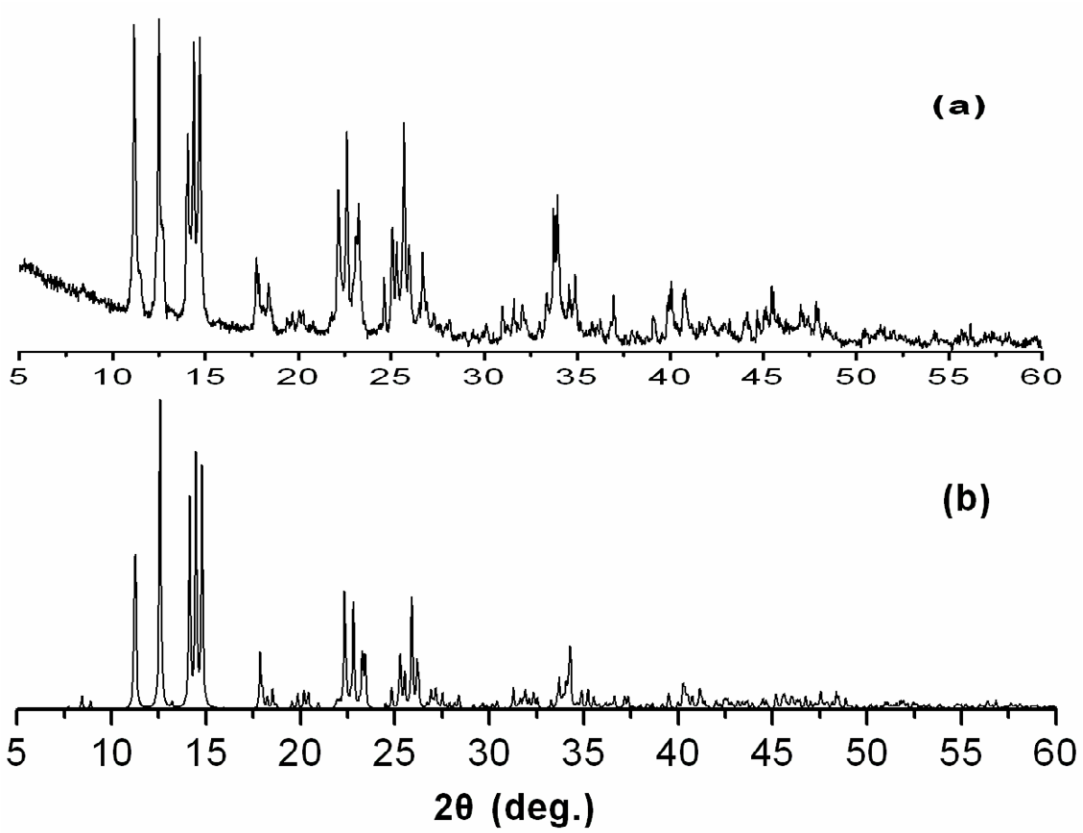

Figure S6: Powder XRD patterns of **1**: (a) Experimental powder X-ray diffraction pattern; (b) simulated from single crystal X-ray data.

7. Fluorescence excitation spectra and emission spectra of **1** in the solid state.

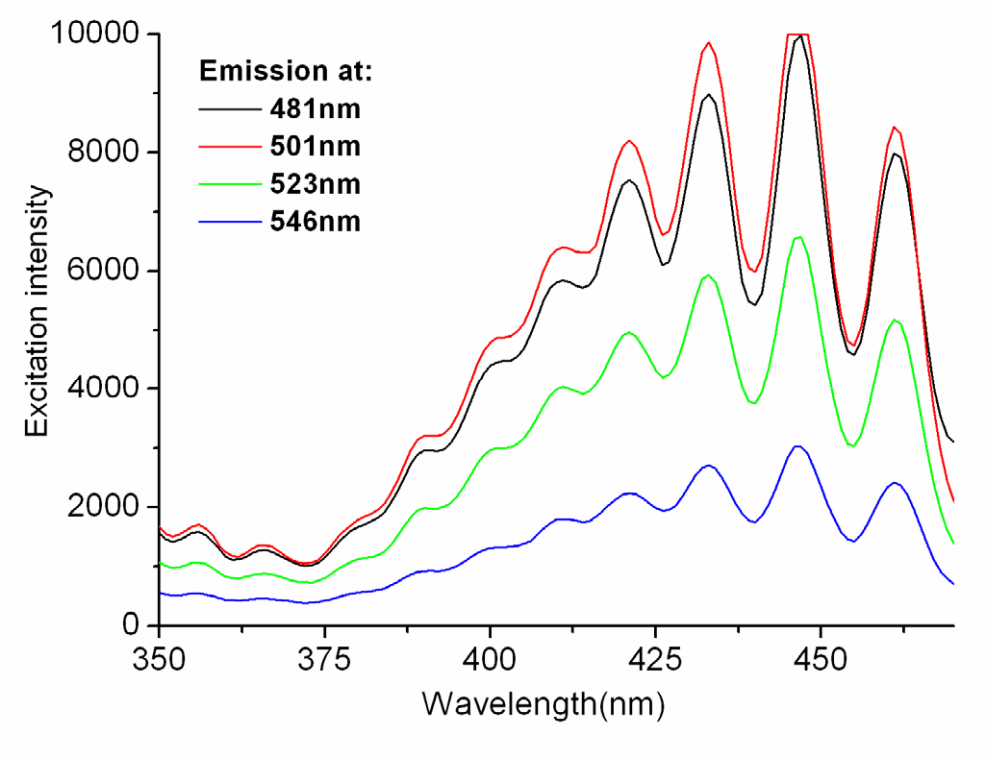

Figure S7-1 Solid-state excitation spectra for **1** at different emission wavelengths at RT.

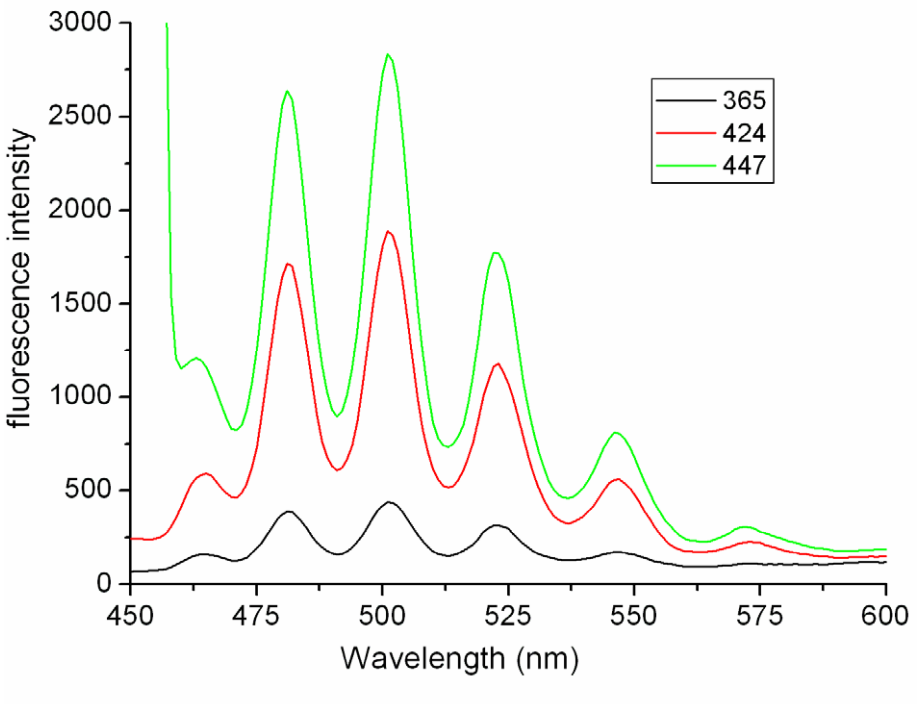

Figure S7-2 Solid-state emission spectra for **1** at different excitation wavelengths at RT.