Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Three Sandwich-type Zinc(II)-Lanthanide(III) Clusters: Structures, Luminescence and Magnetic properties

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Table S1. Crystal data and structure refinement parameters for compound $Zn^{II}_2Eu^{III}_4$, $Zn^{II}_2Tb^{III}_4$ and $Zn^{II}_2Dy^{III}_4$.

	$Zn^{II}_2Eu^{III}_4$	$Zn^{II}_2Tb^{III}_4$	$Zn^{II}_2Dy^{III}_4$
Empirical formula	$Zn_2Eu_4C_{94}H_{114}N_{10}O_{42}$	$Zn_2Tb_4C_{94}H_{114}N_{10}O_{42}$	$Zn_2Dy_4C_{94}H_{114}N_{10}O_{42}$
Formula weight	2794.62	2822.46	2836.74
Temperature	293(2)	293(2)	293(2)
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 16.6693(5)Å	a = 16.5858(3)Å	a = 16.513(3)Å
	b = 17.1718(5) Å	b = 17.2083(3) Å	b = 17.241(3) Å
	c = 20.9256(7) Å	c = 21.1240(4) Å	c = 23.807(8) Å
	β = 102.3553˚	β = 102.2803˚	β = 120.282˚
Volume (Å^3), Z	5851.1(13), 2	5891.11(91), 2	5853(3), 2
Absorption coefficient	2.599 mm^{-1}	2.853 mm^{-1}	3.008 mm^{-1}
F(000)	2792	2808	2816
ϑ range for data collection	3.69 to 26.01	3.47 to 25.50	3.45 to 25.50
Limiting indices	-20 ≤ h ≤ 16	-9 ≤ h ≤ 20	-19 ≤ h ≤ 20
	-21 ≤ k ≤ 19	-20 ≤ k ≤ 12	-20 ≤ k ≤ 19
	-25 ≤ l ≤ 22	-25 ≤ l ≤ 25	-25 ≤ l ≤ 28
R_{int}	0.0523	0.0577	0.0682
Reflections collected unique	21584/11508	21520/10920	25663/10859
Completeness	99.7 %	99.8 %	99.8 %
Absorption correction	Multi-Scan	Multi-Scan	Multi-Scan
Data/restraints /parameters	11508 / 828 /695	10920/861/698	10859/86/697
Goodness-of-fit on F^2	1.040	1.05	1.048
Final R indices [I>2sigma(I)]	R_1 = 0.0571, wR_2 = 0.2349	R_1 = 0.0577, wR_2 =0.1685	R_1 = 0.0682, wR_2 =0.1524
R indices (all data)	R_1 = 0.1419, wR_2 = 0.1711	R_1 = 0.1480, wR_2 =0.1711	R_1 = 0.0873, wR_2 =0.1623
Largest diff. peak and hole	2.231 and -1.260 (e·Å^{-3})	2.368 and -1.366(e·Å^{-3})	3.286 and -4.505(e·Å^{-3})

Table S2. Important bond lengths for compound $Zn^{II}_2Eu^{III}_4$, $Zn^{II}_2Tb^{III}_4$ and $Zn^{II}_2Dy^{III}_4$.

$[Zn_2Eu_4(HL)_4(o\text{-Vanilline})_2(OH)_4]2NO_3{\cdot}4CH_3OH$ ($Zn^{II}_2Eu^{III}_4$)									
Eu1–O15	2.345(5)	Eu1–O14	2.358(5)	Eu1–O3	2.375(6)	Eu1–O2	2.376(6)	Eu1–O15	2.384(5)
Eu1–O11	2.399(6)	Eu1–O16	2.416(6)	Eu1–O12	2.439(5)	Eu2–O7	2.242(6)	Eu2–O15	2.378(5)
Eu2–O8	2.382(6)	Eu2–O9	2.396(6)	Eu2–O12	2.447(5)	Eu2–O14	2.496(5)	Eu2–O2	2.496(5)
Eu2–O13	2.655(6)	Zn1–O14	2.002(6)	Zn1–O4	2.072(6)	Zn1–N4	2.074(7)	Zn1–N2	2.091(7)
Zn1– O9	2.100(6)								
$[Zn_2Tb_4(HL)_4(o\text{-Vanilline})_2(OH)_4]2NO_3{\cdot}4CH_3OH$ ($Zn^{II}_2Tb^{III}_4$)									
Tb–O4	2.211(6)	Tb–O14	2.352(6)	Tb–O2	2.360(6)	Tb–O3	2.362(6)	Tb–O11	2.408(6)
Tb–O7	2.467(6)	Tb–O16	2.485(6)	Tb–O12	2.650(6)	Tb2–O14	2.301(6)	Tb2–O16	2.327(6)
Tb2–O8	2.341(6)	Tb2–O7	2.347(6)	Tb2–O13	2.371(6)	Tb2–O14	2.376(5)	Tb2–O15	2.392(6)
Tb2–O11	2.421(6)	Zn–O16	2.001(6)	Zn1–N1	2.071(8)	Zn–O9	2.072(6)	Zn–N4	2.098(8)
Zn1–O2	2.109(6)								
$[Zn_2Dy_4(HL)_4(o\text{-Vanilline})_2(OH_)_4]2NO_3{\cdot}4CH_3OH$ ($Zn^{II}_2Dy^{III}_4$)									
Dy–O11	2.301(6)	Dy–O15	2.322(6)	Dy1–O7	2.343(6)	Dy–O8	2.352(6)	Dy–O11	2.353(6)
Dy–O13	2.354(6)	Dy1–O16	2.377(6)	Dy1–O12	2.422(6)	Dy2–O2	2.189(7)	Dy2–O1	2.333(7)
Dy2–O11	2.345(6)	Dy2–O4	2.359(6)	Dy2–O12	2.385(6)	Dy2–O15	2.458(6)	Dy2–O7	2.460(7)
Dy2–O14	2.645(6)	Zn1–O15	2.004(6)	Zn1–N2	2.058(9)	Zn–N4	2.071(8)	Zn–O9	2.084(7)
Zn1–O4	2.101(7)								

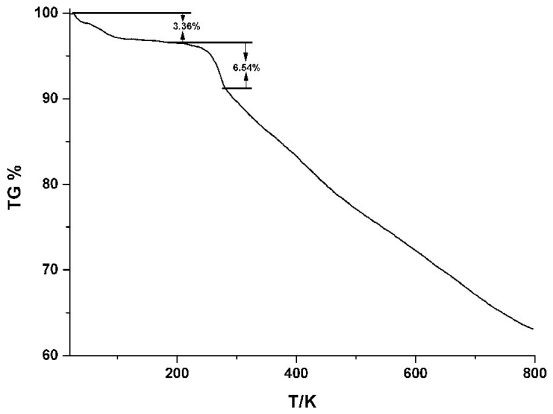

Figure S1. TG curves for $Zn^{II}_2Dy^{III}_4$.

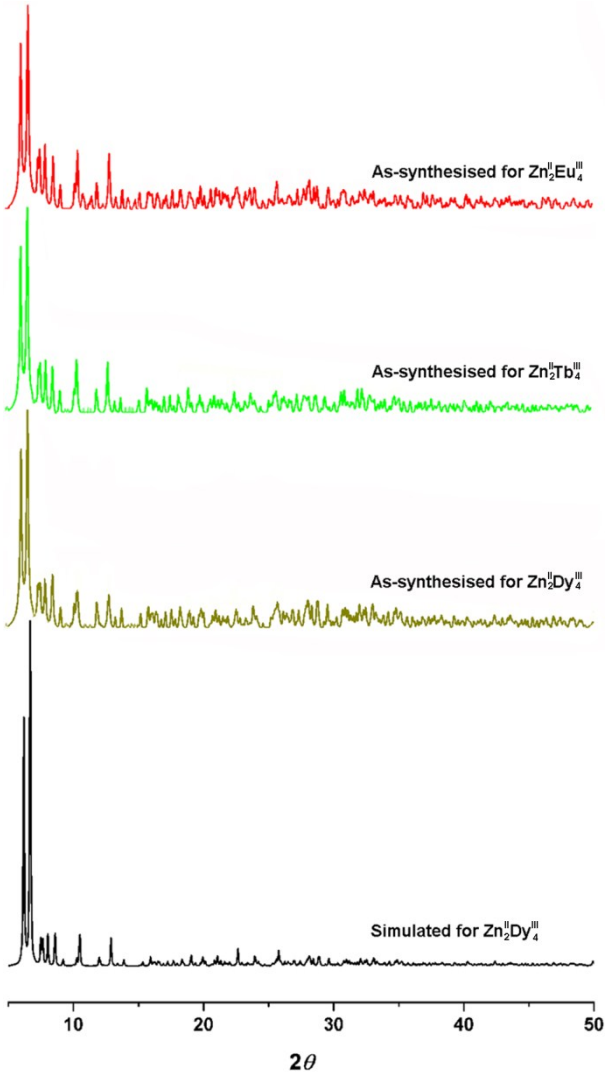

Figure S2. Comparing the simulated PXRD (black) and experimental patterns of compounds $Zn^{II}_2Eu^{III}_4$, $Zn^{II}_2Tb^{III}_4$ and $Zn^{II}_2Dy^{III}_4$.

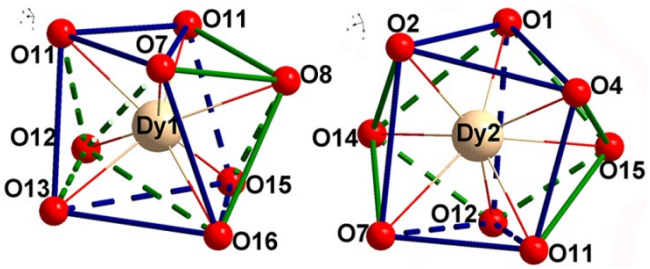

Figure S3 Coordination polyhedron of Dy^{III} in $Zn^{II}_2Dy^{III}_4$.

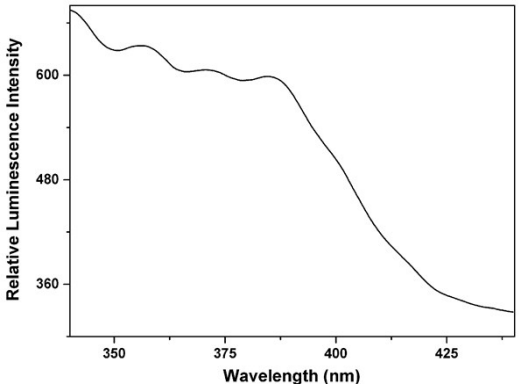

Figure S4 Excitation spectra of $Zn^{II}_2Eu^{III}_4$ at room temperature.

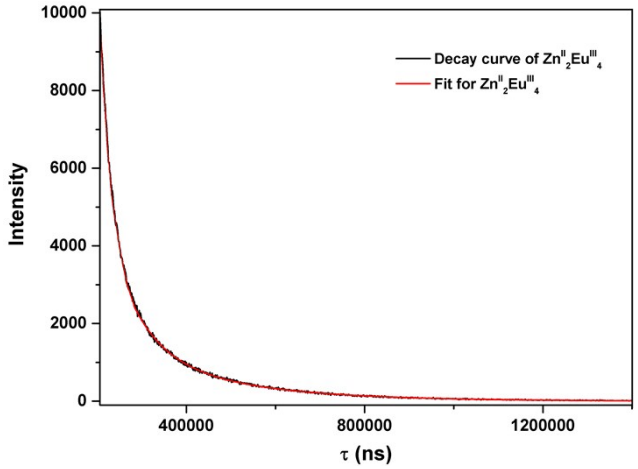

Figure S5 Emission decay curves of $Zn^{II}_2Eu^{III}_4$.

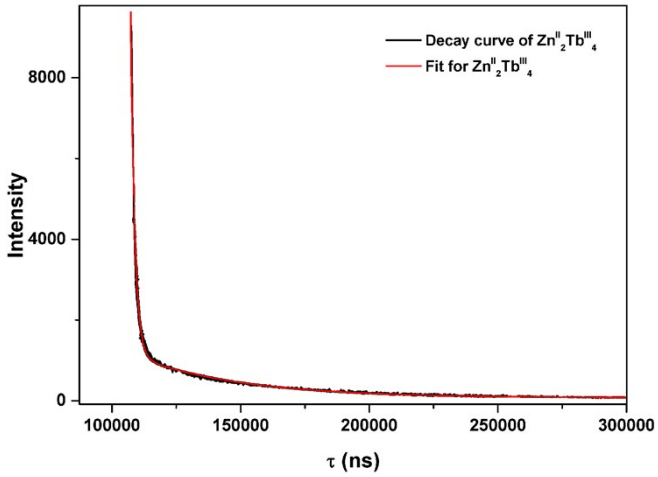

Figure S6 Emission decay curves of $Zn^{II}_2Tb^{III}_4$.

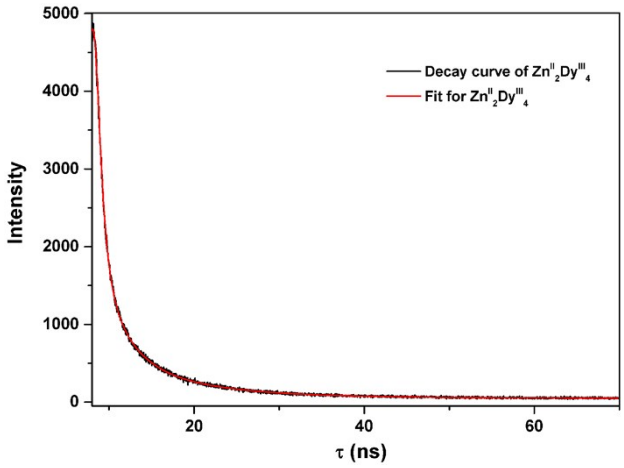

Figure S7 Emission decay curves of $Zn^{II}_2Dy^{III}_4$.

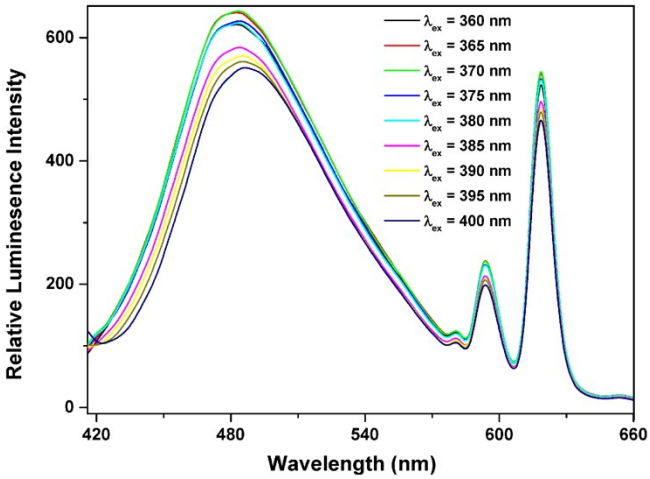

Figure S8 Emission spectra of different wavelength exciation for $Zn^{II}_2Eu^{III}_4$.

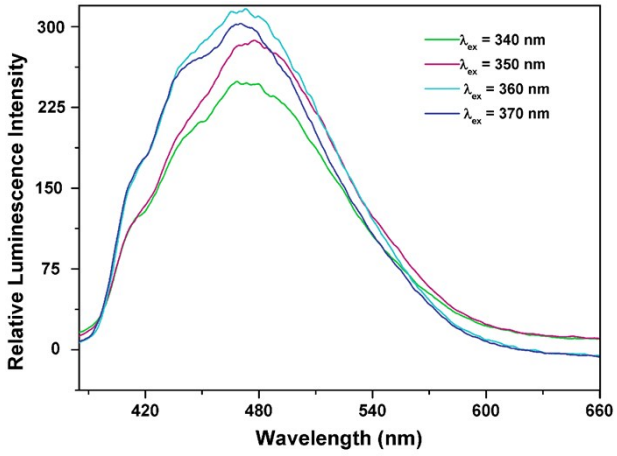

Figure S9 Emission spectra of different wavelength exciation for $Zn^{II}_2Tb^{III}_4$.

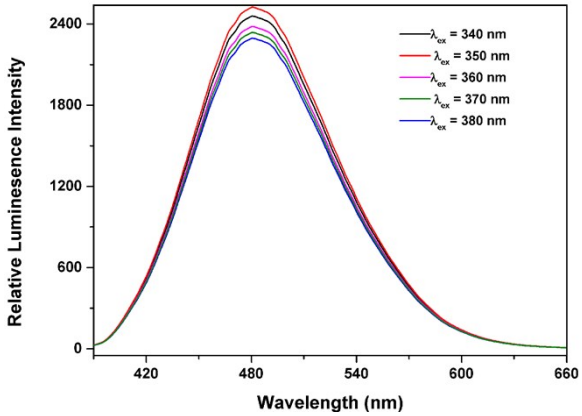

Figure S10 Emission spectra of different wavelength exciation for $Zn^{II}_2Dy^{III}_4$.