Supplementary Information

Fluorescence Property and Density Functional Theory Calculation of Structurally Characterized Heterotetranuclear [Zn^{II}_2-Sm^{III}_2] 4,4′-Bipy-Salamo-Constructed Complex

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1. X-ray Crystallography analysis

The diffraction intensity data of the [Zn^{II}_2-Sm^{III}_2] complex was collected by a Bruker APEX-II CCD surface detector diffractometer, and the Mo-Kα ray radiation was monochromated with a graphite monochromator, and the diffrn radiaction wavelength λ = 0.71073 Å. At a temperature of 273(2) K, several independent diffraction spots were scanned and collected by scanning with φ and ω, and reduction and refinement of the obtained diffraction data were applied to the SAINT program [1]. The crystal structure was resolved using the ShelXTL 2015 program [2], reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement. All non-hydrogen atoms were found by number theory Fourier synthesis, while hydrogen atoms were obtained by geometric hydrogenation. The crystallographic data of the [Zn^{II}_2-Sm^{III}_2] complex was collected and stored in the Cambridge Crystallography Data Center. The deposit number is CCDC 1959376, and specific data for this crystal structure can be obtained from the Cambridge Crystallographic Data Center at www.ccdc.cam.ac.uk/conts/retrieving.html.

2. IR Spectra

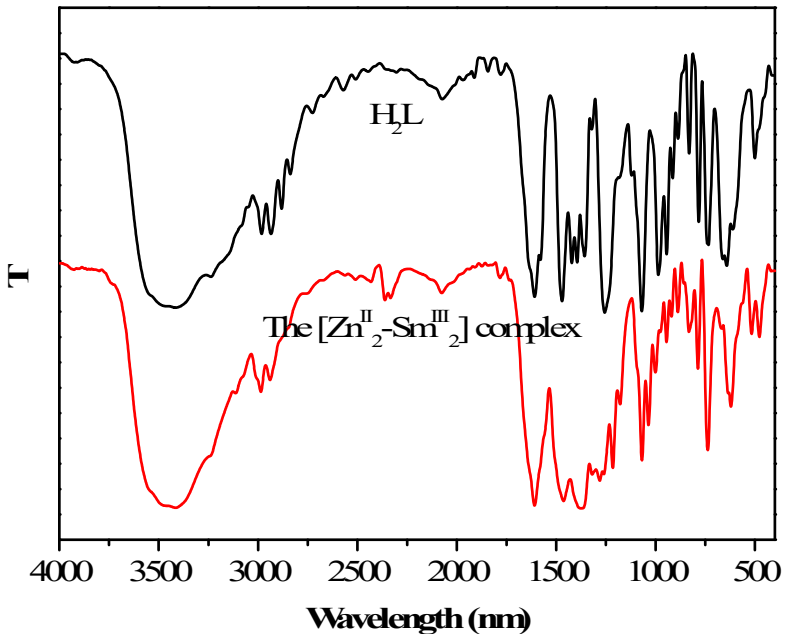

Figure S1. Infrared Spectra of H_2L and the [Zn^{II}_2-Sm^{III}_2] complex.

3. Crystal Structure and Supra-molecular Interactions

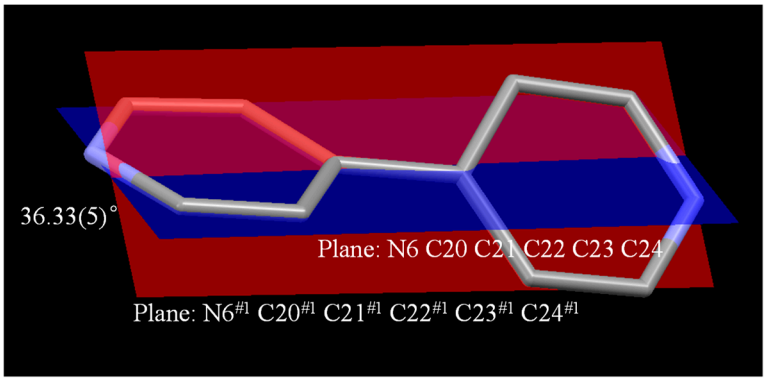

Figure S2. The dihedral angle between the planes of the two pyridine rings of the [Zn^{II}_2-Sm^{III}_2] complex.

Table S1. Essential bond lengths (Å) and angles (°) of the [Zn^{II}_2-Sm^{III}_2] complex.

Bond	Lengths	Bond	Lengths
Sm1-O1	2.630(3)	Sm1-O14	2.539(3)
Sm1-O2	2.351(3)	Sm1-N3	2.961(4)
Sm1-O5	2.390(3)	Sm1-N4	2.062(4)
Sm1-O6	2.594(3)	Zn1-O2	2.076(5)
Sm1-O7	2.601(3)	Zn1-O5	2.035(3)
Sm1-O8	2.475(3)	Zn1-N6	2.068(3)
Sm1-O10	2.552(4)	Zn1-N1	2.127(4)
Sm1-O11	2.481(3)	Zn1-N2	2.036(3)
Sm1-O13	2.560(3)		
Bond	**Angles**	**Bond**	**Angles**
O1-Sm1-N2	132.20(11)	O8-Sm1-N4	71.49(12)
O1-Sm1-N4	72.89(11)	O10-Sm1-O1	70.36(11)
O2-Sm1-O1	62.14(9)	O10-Sm1-O6	133.49(11)
O2-Sm1-O5	66.19(9)	O10-Sm1-O7	66.39(12)
O2-Sm1-O6	127.36(10)	O10-Sm1-O13	143.75(12)

O2-Sm1-O7	75.76(10)	O10-Sm1-N3	66.42(12)
O2-Sm1-O8	125.40(10)	O10-Sm1-N4	25.12(11)
O2-Sm1-O10	93.34(10)	O11-Sm1-O1	78.22(11)
O2-Sm1-O11	134.31(11)	O11-Sm1-O6	97.97(11)
O2-Sm1-O13	79.75(10)	O11-Sm1-O7	105.08(11)
O2-Sm1-O14	121.07(11)	O11-Sm1-O10	50.07(11)
O2-Sm1-N3	100.71(11)	O11-Sm1-O13	112.43(10)
O2-Sm1-N4	114.88(11)	O11-Sm1-O14	64.16(11)
O5-Sm1-O1	122.09(10)	O11-Sm1-N3	89.08(12)
O5-Sm1-O6	62.64(9)	O11-Sm1-N4	24.96(11)
O5-Sm1-O7	72.44(11)	O13-Sm1-O1	75.08(11)
O5-Sm1-O8	89.18(12)	O13-Sm1-O6	73.63(11)
O5-Sm1-O10	137.52(11)	O13-Sm1-O7	142.42(11)
O5-Sm1-O11	158.94(11)	O13-Sm1-N3	149.77(12)
O5-Sm1-O13	71.75(10)	O13-Sm1-N4	131.08(11)
O5-Sm1-O14	112.57(11)	O14-Sm1-O1	75.75(12)
O5-Sm1-N3	80.76(11)	O14-Sm1-O6	70.74(12)
O5-Sm1-N4	157.09(11)	O14-Sm1-O7	163.18(11)
O6-Sm1-O1	144.12(11)	O14-Sm1-O10	109.87(11)
O6-Sm1-O7	99.49(11)	O14-Sm1-O13	49.53(10)
O6-Sm1-N3	82.85(11)	O14-Sm1-N3	138.17(12)
O6-Sm1-N4	116.93(11)	O14-Sm1-N4	86.99(12)
O7-Sm1-O1	116.06(11)	N3-Sm1-N4	76.56(12)
O7-Sm1-N3	25.03(10)	O2-Zn1-N6	99.12(12)
O7-Sm1-N4	85.48(12)	O2-Zn1-N1	84.76(12)
O8-Sm1-O1	142.55(12)	O2-Zn1-N2	156.41(13)
O8-Sm1-O6	65.86(12)	O5-Zn1-O2	79.15(11)
O8-Sm1-O7	49.99(10)	O5-Zn1-N6	113.79(13)
O8-Sm1-O10	72.51(12)	O5-Zn1-N1	145.34(13)
O8-Sm1-O11	74.46(12)	O5-Zn1-N2	86.82(13)
O8-Sm1-O13	139.48(12)	N6-Zn1-N1	98.88(14)
O8-Sm1-O14	113.26(11)	N2-Zn1-N6	103.89(14)
O8-Sm1-N3	24.98(10)	N2-Zn1-N1	96.66(14)

References

1. Madison, W.I. SAINT-Plus, Bruker Analytical X-ray System; Bruker: Billerica, MA, USA, **1999**.

2. Sheldrick, G.M. Acta Crystallogr. Sect. C: Cryst. Struct. Commun. **2015**, C71, 3–8.