Supporting Information

Construction of Homochiral Alkaline-lanthanide Heteronuclear Helicates with Na^+-selective Bonding in Self-assembly Process

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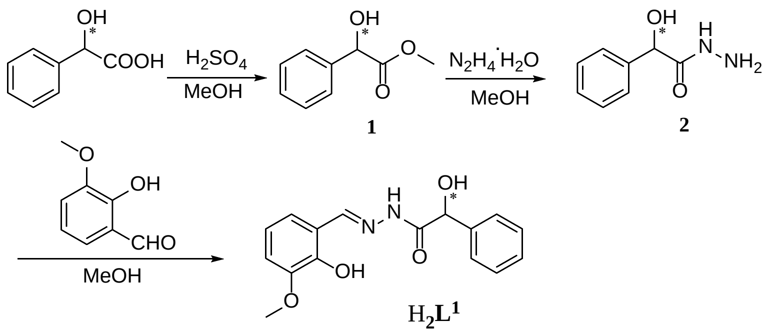
Synthesis of the ligand



Scheme S1. Preparation of ligand H_2**L**[1].

Methyl mandelate (1).

Mandelic acid (9.0 g, 0.059 mol) was dissolved in methanol (200 ml) and was slowly added with concentrated sulfuric acid (1.5 ml). After the reaction, adjusted pH = 7-8 with saturated aqueous $NaHCO_3$ solution, and extracted with ethyl acetate. The organic phase solvent was removed in vacuo and placed in freezer to give a white solid **1**. (9.5 g, yield 97%).

2-hydroxy-2-phenylacetohydrazide (2)

Methyl mandelate (9.5 g, 0.057 mol) was dissolved in methanol (200 ml) and added with $N_2H_4 \cdot H_2O$ (3.7 g). After refluxed for 12 hours, the solvent was removed in vacuo and obtain a white solid **2**. (9.4 g, yield 98%).

Ligand H_2**L**[1]

2-hydroxy-2-phenylacetohydrazide (9.4 g, 0.056 mol) was dissolved in 200 ml methanol and added with 2-hydroxy-3-methoxybenzaldehyde (8.6 g, 0.057 mol). The solution was refluxed for 12 h and removed the solvent in vacuo to obtain a yellow powder (15 g, yield 94.6%).

Ligand H_2**L**[2]

The synthesis of ligand H_2**L**[2] was the same as H_2**L**[1] except that

2-hydroxy-3-methoxybenzaldehyde was substituted for salicylaldehyde.

S-H_2**L**[1]

$[\alpha]_D^{20}$ = -35 $cm^3\ g^{-1}\ dm^{-1}$(c = 0.002 g cm^{-3}, methanol). ^{1}H-NMR (400 MHz, CD_3OD) δ 8.50 (s, 1H), 7.54 – 7.46 (m, 2H), 7.38 – 7.27 (m, 3H), 7.07 (dd, J = 8.0, 1.5 Hz, 1H), 6.96 (dd, J = 8.1, 1.6 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 5.17 (s, 1H), 3.82 (s, 3H). ^{13}C-NMR (400 MHz, DMSO-D6) δ 56.19, 73.85, 114.12, 119.03, 119.41, 121.40, 127.02, 128.15, 128.67, 141.05, 147.42, 148.36, 149.26, 169.09. ESI-MS m/z: calcd. for $C_{16}H_{16}N_2O_4$ 300.1, found:301.1 $[M+H]^+$.

R-H_2**L**[1]

$[\alpha]_D^{21}$ = +35 $cm^3\ g^{-1}\ dm^{-1}$(c = 0.002 g cm^{-3}, methanol). ^{1}H-NMR (400 MHz, CD_3OD) δ 8.51(s, 1H), 7.53-7.4(m, 3H), 7.3-7.28(m, 4H), 7.08(dd, J = 7.9, 1.5Hz, 1H), 6,98 (dd, J = 8.0, 1.4Hz, 1H), 5.17 (s, 1H), 3.83 (s, 3 H). ^{13}C-NMR (400 MHz, DMSO-D6) δ 56.42, 73.91, 114.45, 119.24, 119.40, 121.53, 127.01, 128.16, 128.50, 141.07, 147.69, 148.40, 149.39, 169.10. ESI-MS m/z: calcd. for $C_{16}H_{16}N_2O_4$ 300.1, found:301.1 $[M+H]^+$.

S-H_2**L**[2]

$[\alpha]_D^{21}$ = -40 $cm^3\ g^{-1}\ dm^{-1}$(c = 0.002 g cm^{-3}, methanol).^{1}H-NMR (400 MHz, CD_3OD) δ 8.45 (s, 1H), 7.61–7.43 (m, 2H), 7.39–7.20 (m, 5H), 6.86 (dtt, J = 7.9, 5.2, 2.6 Hz, 2H), 5.18 (s, 1H). ^{13}C-NMR (400 MHz, CD_3OD) δ 73.76, 115.81, 117.70, 119.28, 125.73, 128.41, 129.99, 131.09, 139.52, 151.01, 157.55, 170.15. ESI-MS m/z: calcd. for $C_{15}H_{14}N_2O_3$ 270.1.1, found:271.1 $[M+H]^+$

R-H_2**L**[2]

$[\alpha]_D^{21}$ = +40 $cm^3\ g^{-1}\ dm^{-1}$(c = 0.002 g cm^{-3}, methanol). ^{1}H-NMR (400 MHz, CD_3OD) δ 8.46 (s, 1H), 7.54 – 7.43 (m, 3H), 7.43 – 7.20 (m, 8H), 6.92 – 6.79 (m, 3H), 5.18 (s, 1H). ^{13}C-NMR (400 MHz, CD_3OD) δ 73.72, 116.18, 117.74, 119.15, 126.55, 127.78, 128.159, 130.43, 139.60, 151.02, 158.05, 170.24. ESI-MS m/z: calcd. for $C_{15}H_{14}N_2O_3$ 270.1.1, found:271.1 $[M+H]^+$.

Synthesis of Complexes

$[Dy_2Na_3\{(S)\text{-}HL^1\}_6]\cdot 3NO_3\cdot$solvent ***(1a)***

(*S*)-H_2**L**[1](0.06 mmol, 0.0180g) was added into 1 ml methanol solution of NaOH (0.1 M) and added with 2 ml acetonitrile. After the mixture had been stirred for 3 min, 0.03 mmol $Dy(NO_3)_3\cdot 6H_2O$(0.0137 g) was added. Then, the solution was stirred for 3 min until obtain a clearly yellow solution. The crystals of complex **1a** suitable for single-crystal X-ray diffraction analysis were obtained 47% yield by slow evaporation of the solution with one week at room temperature in air. Elemental analysis for complex **1a** $C_{96}H_{90}Dy_2N_{15}Na_3O_{33}$ (non-coordinated solvent molecules were lost by drying): C, 47.68; H, 3.71; N, 8.60 (calculated: C, 48.48; H, 3.79; N, 8.83.) IR (KBr, *υ*, cm^{-1}): 3199(m), 3028(w), 2835(w), 1604(s), 1541(m), 1454(s), 1380(s), 1296(m), 1218(s), 1082(m), 948(w), 848(m), 732(s), 694(m), 619(w).

$[Dy_2Na_3\{(R)\text{-}HL^1\}_6]\cdot 3NO_3\cdot$solvent ***(1b)***

The synthesis steps of enantiomer complex **1b** was the same procedure as that for complex **1a**, except that (*R*)-H_2**L**[1] instead of (*S*)-H_2**L**[1]. The crystals of complex **1b** suitable for single-crystal X-ray diffraction analysis were obtained 45% yield by slow evaporation of the solution with one week at room temperature in air. Elemental analysis for complex **1b** $C_{96}H_{90}Dy_2N_{15}Na_3O_{33}$ (non-coordinated solvent molecules were lost by drying): C, 47.78; H, 3.65; N, 8.71 (calculated: C, 48.48; H, 3.79; N, 8.83.) IR (KBr, υ, cm^{-1}): 3446(w), 3033(w), 1602(s), 1546(w), 1448(s), 1380(s), 1296(m), 1082(m), 947(w), 852(w), 742(s), 694(w), 621(w).

*[Dy₄(μ₄-OH) {(S)-HL²}₈]·3NO₃·MeOH·4H₂O (**2a**)*

The synthesis steps of complex **2a** was the same procedure as that for complex **1a**, except that (*S*)-H_2**L**^{2} instead of (*S*)-H_2**L**^{1}. Elemental analysis for complex **2a** $C_{120}H_{105}Dy_4N_{19}O_{34}$ (non-coordinated solvent molecules were lost by drying): C, 46.65; H, 3.68; N, 8.69 (calculated: C, 47.58; H, 3.57; N, 8.79.) IR (KBr, υ, cm^{-1}): 3296(m), 3037(w), 1631(s), 1604(s), 1544(m), 1471(m), 1438(m), 1379(s), 1319(w), 1284(s), 1199(m), 1155(w), 1066(w), 960(w), 896(m), 759(m), 732(m), 694(m), 586(w), 511(w).

*$[Dy_4(\mu_4\text{-}OH)\{(R)\text{-}H\mathbf{L}^2\}_8]\cdot 3NO_3\cdot 2CH_3CN\cdot 6H_2O$ (**2b**)*

The synthesis steps of complex **2b** was the same procedure as that for complex **1a**, except that (*R*)-H_2**L**^{2} instead of (*S*)-H_2**L**^{1}. Elemental analysis for complex **2b** $C_{120}H_{105}Dy_4N_{19}O_{34}$ (non-coordinated solvent molecules were lost by drying): C, 46.81; H, 3.72; N, 8.73 (calculated: C, 47.58; H, 3.57; N, 8.79.) IR (KBr, υ, cm^{-1}): 3290(m), 3031(w), 1641(s), 1608(s), 1544(m), 1471(m), 1438(m), 1380(s), 1319(w), 1284(s), 1197(w), 1149(w), 1060(w), 894(w), 757(m), 732(m), 694(w), 588(w), 511(w).

Mixed-metal Self-assembly Experiments

In this work, (*S*)-H_2**L**^{1} was used as an example to illustrate the Na^+-selective bonding in self-assembly process. (*S*)-H_2**L**^{1}(0.06 mmol, 0.0180g) dissolved in 3 ml acetonitrile was deprotonated by adding 2 ml methanol solution of KOH (0.1 M) and stirred for 3 min. After the ligand was completely dissolved, 0.03 mmol various metal ions (including Dy^{3+}, Li^+, Na^+, Mg^{2+} and Ca^{2+}, the lanthanide salt is nitrate and the other metal salts is perchlorate) was added, respectively. Then, the solution was stirred for 3 min until obtain a clearly yellow solution. The crystal of complex was obtained by slow evaporation of the solution about two weeks at room temperature in air.

Materials and Methods

All reagents and solvents were purchased from commercial sources and used without further purification. ^{1}H-NMR spectra were recorded on a JNM-ECS-400 MHz spectrometer and referenced to the solvent signals. The infrared spectra were obtained by a Burker VERTEX 70 FT-IR spectrometer using KBr pellets in the range from 400 cm^{-1} to 4000 cm^{-1}. X-ray powder diffraction data of all samples were recorded on a PANalytical X'Pert Pro Diffractometer equipped with Cu Kα radiation (λ =1.5406 Å) and operated at 40 kV and 40 mA with scanning ranges from 3° to 50°. The solution CD spectra were recorded on an Olis DSM 1000 spectropolarimeter. HRESI-MS were performed on Fourier Transform Ion Cyclotron Resonance Mass Spectrometer.

Crystal datas for all complexes were collected on a Bruker FRAMBO diffractometer (**1a** and **2a**: Mo Kα radiation, λ = 0.71073 Å; **1b** and **2b**: Cu Kα radiation, λ = 1.5418 Å). Data reduction was accomplished by the Bruker SAINT program. Structures were solved by direct methods and refined by a full matrix least-squares technique based on F^2 using the Olex2 program. All non-hydrogen atoms were refined anisotropically. For **1a** and **1b**, due to the serious disorder of the solvent molecules, we removed the solvent molecules with SQUEEZE. The details of the crystal parameters, data collections and refinements are summarized in Table S1. Selected bond lengths and angles for all complexes are given in Table S2.

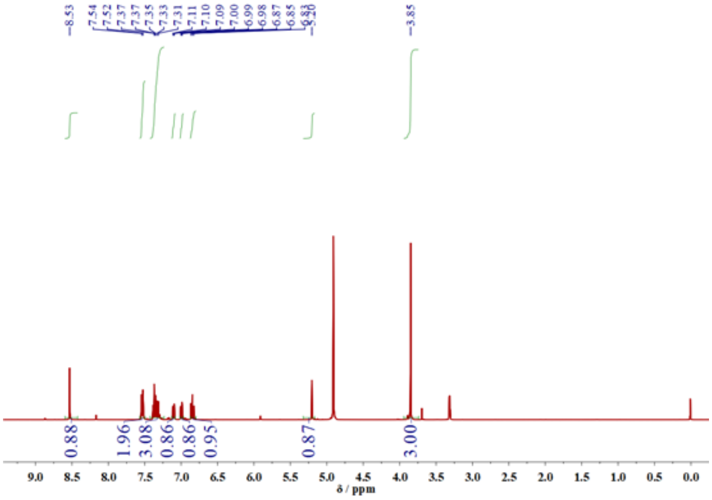


Figure S1 ^{1}H-NMR spectrum (400 MHz, CD_3OD) of ligand (*S*)-H_2**L**^{1}.

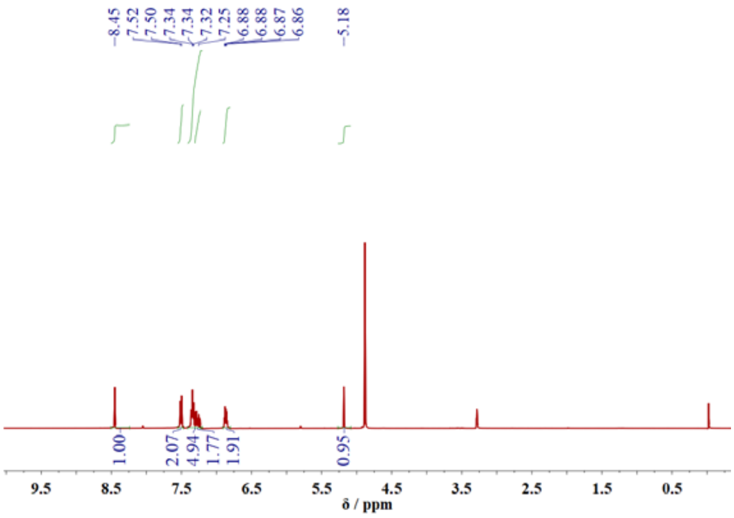


Figure S2 ^{1}H-NMR spectrum (400 MHz, CD_3OD) of ligand (*S*)-H_2**L**^{2}.

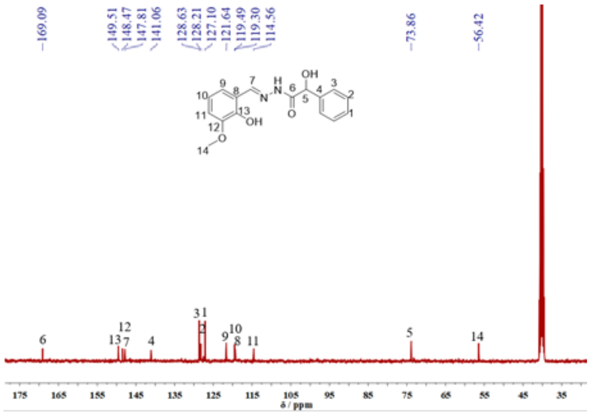


Figure S3 ^{13}C-NMR (400 MHz, DMSO-d6) spectra of the(*S*)-H_2**L**^{1}.

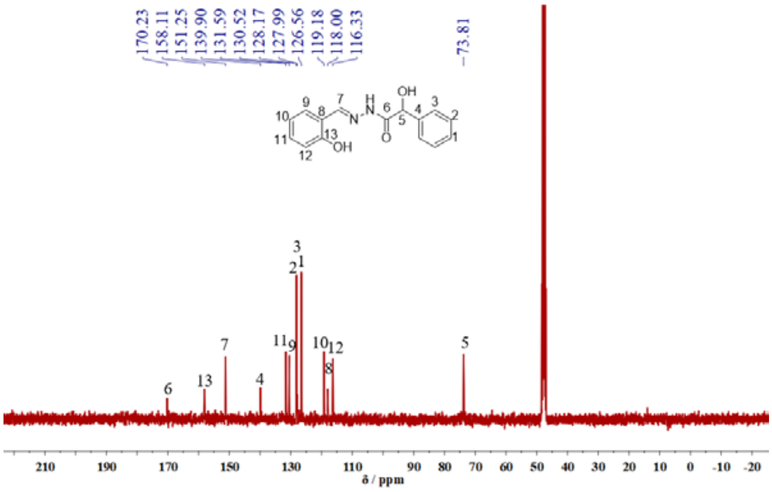


Figure S4 ^{13}C-NMR (400 MHz, CD_3OD) spectra of the(*S*)-H_2**L**^{2}.

Table S1 Crystal Data and Structure Refinement Parameters for Complexes.

	Complex **1a**	Complex **1b**	Complex **2a**	Complex **2b**
Crystal System	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space Group	$C222_1$	$C222_1$	$P2_12_12_1$	$P2_12_12_1$
a (Å)	21.876(6)	20.2482(2)	16.4632(2)	16.5304(4)
b (Å)	20.204(5)	21.6632(2)	21.6760(4)	21.5083(5)
c (Å)	56.153(14)	55.8238(6)	34.7600(6)	34.7813(7)
α (°)	90	90	90	90
β (°)	90	90	90	90
γ (°)	90	90	90	90
Z	8	4	4	4
Volume (Å 3)	24819(11)	24486.6(4)	12404.3(4)	12366.2(5)
ρ_{calc} g/cm^3	1.272	1.391	1.645	1.515
μ (mm^{-1})	1.279	7.271	2.471	13.327
F(000)	9600.0	10408.0	6116.0	5600.0
Temperature	296.15	120.15	100.00(10)	153.15
Reflections collected	61577	42501	85131	92228
Independent ref.	21795	22338	24435	20889
Data/restraints/parameters	21795/211/1340	22338/181/1544	24435/3181/1652	20889/2804/1494
R_{int}	0.0537	0.0313	0.0573	0.0541
Flack parameter	0.071(13)	-0.0013(16)	-0.009(5)	0.049(4)
Final R indices [I>2.0σ(I)]	R1 = 0.0596, wR2 = 0.1323	R1 = 0.0461, wR2 = 0.1261	R_1 = 0.0582, wR_2 = 0.1479	R_1 = 0.0360, wR_2 = 0.0929
Final R indexes [all data]	R1 = 0.0640, wR2 = 0.1342	R1 = 0.0495, wR2 = 0.1284	R_1 = 0.0763, wR_2 = 0.1618	R_1 = 0.0375, wR_2 = 0.0938
GOF	1.098	1.065	1.041	1.021

Table S2 Selected Bond Lengths (Å) and Angles (°) for All Complexes.

Complex **1a**							
Dy(1)-O(2)	2.312(7)	Na(1)-O(7)	2.315(9)	Na(2)-O(3)1	2.290(8)	Na(4)-O(14)	2.323(9)
Dy(1)-O(1)	2.328(7)	Na(1)-O(2)	2.300(8)	Dy(2)-O(15)	2.322(8)	Na(4)-O(15)	2.544(9)
Dy(1)-O(3)	2.319(7)	Na(1)-O(1)1	2.297(9)	Dy(2)-O(23)	2.385(8)	Na(4)-O(15)2	2.309(9)
Dy(1)-O(8)	2.437(7)	Na(1)-O(1)	2.587(8)	Dy(2)-O(17)	2.427(9)	Na(4)-O(16)2	2.334(9)
Dy(1)-O(11)	2.371(8)	Na(1)-O(3)1	2.615(8)	Dy(2)-O(20)	2.404(8)	Na(3)-O(13)	3.109(1)
Dy(1)-O(5)	2.433(8)	Na(2)-O(4)	2.321(9)	Dy(2)-N(9)	2.601(9)	Na(3)-O(13)2	2.316(9)
Dy(1)-N(3)	2.627(8)	Na(2)-O(4)1	2.321(9)	Dy(2)-N(7)	2.599(1)	Na(3)-O(22)2	2.316(9)
Dy(1)-N(1)	2.584(10)	Na(2)-O(2)	2.589(8)	Dy(2)-N(11)	2.594(9)	Na(3)O(22)	2.339(1)
Dy(1)-N(5)	2.604(9)	Na(2)-O(2)1	2.589(8)	Na(4)-O(19)	2.330(9)	Na(3)-O(14)2	2.339(1)
Na(1)-O(10)1	2.333(8)	Na(2)-O(3)	2.290(8)	Na(4)-O(13)2	2.581(9)	Na(3)-O(14)	2.537(9)
Dy(2)-O(13)	3.105(11)	Dy(2)-O(14)	2.308(8)				

O(2)-Dy(1)-O(1)	80.8(2)	O(13)-Dy(2)-O(23)	130.7(3)	N(5)-Dy(1)-N(3)	119.1(3)
O(2)-Dy(1)-O(3)	81.3(3)	O(13)-Dy(2)-O(17)	141.5(3)	O(10)1-Na(1)-O(1)	90.7(3)
O(2)-Dy(1)-O(8)	129.3(3)	O(13)-Dy(2)-O(20)	83.0(3)	O(10)1-Na(1)-O(3)1	129.8(3)
O(2)-Dy(1)-O(11)	80.6(3)	O(13)-Dy(2)-N(9)	75.2(3)	O(10)1-Na(1)-C(17)	141.9(3)
O(2)-Dy(1)-O(5)	140.9(3)	O(13)-Dy(2)-N(7)	141.0(3)	O(10)1-Na(1)-C(33)1	48.9(3)
O(2)-Dy(1)-N(3)	67.3(3)	O(13)-Dy(2)-N(11)	68.4(3)	O(7)-Na(1)-O(10)1	97.6(3)
O(2)-Dy(1)-N(1)	142.1(3)	O(14)-Dy(2)-O(13)	79.5(3)	O(7)-Na(1)-O(1)	127.4(3)
O(2)-Dy(1)-N(5)	73.8(3)	O(14)-Dy(2)-O(15)	80.2(3)	O(7)-Na(1)-O(3)1	92.9(3)
O(1)-Dy(1)-O(8)	142.6(3)	O(14)-Dy(2)-O(23)	141.6(3)	O(2)-Na(1)-O(10)1	149.0(3)
O(1)-Dy(1)-O(11)	129.3(3)	O(14)-Dy(2)-O(17)	83.2(3)	O(2)-Na(1)-O(7)	70.9(3)
O(1)-Dy(1)-O(5)	81.2(3)	O(14)-Dy(2)-O(20)	130.2(3)	O(2)-Na(1)-O(1)	75.7(3)
O(1)-Dy(1)-N(3)	141.7(3)	O(14)-Dy(2)-N(9)	68.7(3)	O(2)-Na(1)-O(3)1	80.4(3)
O(1)-Dy(1)-N(1)	74.3(3)	O(14)-Dy(2)-N(7)	74.2(3)	O(2)-Na(1)-C(17)	23.2(3)
O(1)-Dy(1)-N(5)	67.9(3)	O(14)-Dy(2)-N(11)	141.8(3)	O(2)-Na(1)-C(33)1	147.6(3)
O(3)-Dy(1)-O(1)	81.6(3)	O(15)-Dy(2)-O(13)	80.4(3)	O(1)1-Na(1)-O(10)1	70.6(3)
O(3)-Dy(1)-O(8)	82.1(3)	O(15)-Dy(2)-O(23)	82.6(3)	O(1)1-Na(1)-O(7)	150.0(3)
O(3)-Dy(1)-O(11)	140.3(3)	O(15)-Dy(2)-O(17)	130.0(3)	O(1)1-Na(1)-O(2)	132.3(3)
O(3)-Dy(1)-O(5)	129.5(3)	O(15)-Dy(2)-O(20)	141.5(3)	O(1)1-Na(1)-O(1)	81.3(3)
O(3)-Dy(1)-N(3)	73.4(3)	O(15)-Dy(2)-N(9)	143.2(3)	O(1)-Na(1)-O(3)1	120.3(3)
O(3)-Dy(1)-N(1)	67.4(3)	O(15)-Dy(2)N(7)	67.3(3)	O(1)1-Na(1)-O(3)1	76.1(3)
O(3)-Dy(1)-N(5)	143.0(3)	O(15)-Dy(2)-N(11)	74.8(3)	O(4)-Na(2)-O(4)1	96.6(4)
O(8)-Dy(1)-N(3)	62.1(3)	O(23)-Dy(2)-O(17)	82.1(3)	O(4)1-Na(2)-O(2)1	129.4(3)
O(8)-Dy(1)-N(1)	68.4(3)	O(23)-Dy(2)-O(20)	82.4(3)	O(4)-Na(2)-O(2)	129.4(3)
O(8)-Dy(1)-N(5)	134.9(3)	O(23)-Dy(2)-N(9)	134.2(3)	O(4)1-Na(2)-O(2)	91.7(2)
O(11-)Dy(1)-O(8)	82.6(3)	O(23)-Dy(2)-N(7)	67.6(3)	O(4)-Na(2)-O(2)1	91.7(2)
O(11)-Dy(1)-O(5)	84.5(3)	O(23)-Dy(2)-N(11)	62.6(3)	O(2)1-Na(2)-O(2)	49.0(3)
O(11)-Dy(1)-N(3)	67.1(2)	O(17)-Dy(2)-N(9)	66.5(3)	O(3)1-Na(2)-O(4)	97.2(3)

O(11)-Dy(1)-N(1)	137.3(3)	O(17)-Dy(2)-N(7)	62.8(3)	O(3)1-Na(2)-O(4)1	97.2(3)
O(11)-Dy(1)-N(5)	61.7(3)	O(17)-Dy(2)-N(11)	134.9(3)	O(3)-Na(2)-O(4)1	77.9(3)
O(5)-Dy(1)-O(8)	83.7(2)	O(20)-Dy(2)-O(17)	82.4(3)	O(3)-Na(2)-O(4)	77.9(3)
O(5)-Dy(1)-N(3)	137.1(3)	O(20)-Dy(2)-N(9)	61.9(3)	O(3)-Na(2)-O(2)1	112.0(2)
O(5)-Dy(1)-N(1)	62.3(3)	O(20)-Dy(2)-N(7)	135.9(3)	O(3)1-Na(2)-O(2)	112.0(2)
O(5)-Dy(1)-N(5)	67.3(3)	O(20)-Dy(2)-N(11)	66.8(3)	O(3)1-Na(2)-O(2)1	37.52(18)
N(1)-Dy(1)-N(3)	119.6(3)	N(7)-Dy(2)-N(9)	119.2(3)	O(22)-Na(3)-O(14)	126.9(3)
N(1)-Dy(1)-N(5)	120.1(3)	N(11)-Dy(2)-N(9)	119.2(3)	O(22)2-Na(3)-O(14)	92.5(3)
N(11)-Dy(2)-N(7)	119.9(3)	O(15)2-Na(4)-O(13)2	75.5(3)	O(13)-Na(3)-O(22)	70.3(3)
O(19)-Na(4)-O(13)2	-92.2(3)	O(15)2-Na(4)-O(14)	130.7(3)	O(13)-Na(3)-O(14)2	81.8(3)
O(19)-Na(4)-O(15)	126.4(3)	O(15)2-Na(4)-O(15)	80.9(3)	O(13)2-Na(3)-O(14)	81.8(3)
O(19)-Na(4)-O(16)2	98.8(3)	O(15)2-Na(4)-O(16)2	69.9(3)	O(13)-Na(3)-O(14)	75.2(3)
O(14)-Na(4)-O(19)	69.9(3)	O(16)2-Na(4)-O(13)2	125.0(3)	O(13)2-Na(3)-O(14)2	75.2(3)
O(14)-Na(4)-O(13)2	80.8(3)	O(16)2-Na(4)-O(15)	94.1(3)	O(22)2-Na(3)-O(22)	98.1(5)
O(14)-Na(4)-O(15)	75.4(3)	O(13)-Na(3)-O(13)2	132.1(5)	O(22)-Na(3)-O(14)2	92.5(3)
O(14)-Na(4)-O(16)2	153.1(4)	O(13)-Na(3)-O(22)2	150.3(3)	O(22)2-Na(3)O(14)2	126.9(3)
O(15)2-Na(4)-O(19)	151.9(4)	O(13)2-Na(3)-O(22)	150.3(3)	O(22)-Na(3)-O(14)	126.9(3)
O(15)-Na(4)-O(13)2	121.2(3)	O(13)2-Na(3)-O(22)2	70.3(3)	O(22)2-Na(3)-O(14)	92.5(3)

Complex **1b**							
Dy(2)-N(10)	2.587(5)	Dy(2)-N(12)2	2.588(5)	Dy(1)-O(1)	2.389(5)	Dy(1)-O(2)	2.312(4)
Na(2)-O(14)2	2.288(4)	Dy(1)-O(5)	2.424(5)	Na(2)-O(14)	2.289(4)	Dy(1)-O(6)	2.324(5)
Dy(1)-O(9)	2.391(5)	Na(2)-O(15)2	2.315(5)	Dy(1)-O(10)	2.300(4)	Na(2)-O(22)2	2.583(4)
Dy(1)-N(2)	2.586(6)	Na(2)-O(22)	2.583(4)	Dy(1)-N(4)	2.595(6)	Dy(1)-N(6)	2.591(7)
Na(1)-Na(4)	3.422(4)	Na(3)-O(14)	2.607(5)	Na(1)-O(2)	2.583(5)	Na(3)-O(18)	2.304(5)
Na(1)-O(6)1	2.528(5)	Na(3)-O(18)2	2.584(5)	Na(1)-O(6)	2.311(5)	Na(3)-O(19)	2.320(5)
Na(1)-O(7)	2.355(6)	Na(3)-O(22)	2.283(5)	Na(1)-O(10)	2.328(5)	Na(3)-O(23)	2.327(5)
Na(1)-O(11)1	2.352(5)	Na(4)-O(2)1	2.306(5)	Na(4)-O(2)	2.306(5)	Na(4)-O(3)1	2.342(5)
Na(4)-O(3)	2.342(5)	Na(4)-O(10)1	2.545(5)	Dy(2)-O(13)	2.425(4)	Dy(2)-O(14)	2.307(4)
Dy(2)-O(17)	2.379(5)	Dy(2)-O(18)	2.302(4)	Dy(2)-O(21)	2.432(4)	Dy(2)-O(22)2	2.323(4)
Dy(2)-N(8)	2.591(6)						

O(17)-Dy(2)-O(13)	84.47(16)	O(17)-Dy(2)-O(21)2	82.37(16)	O(17)-Dy(2)-N(8)	137.30(17
O(17)-Dy(2)-N(10)	62.27(17)	O(1)-Dy(1)-O(5)	82.10(17)	O(17)-Dy(2)-N(12)2	67.53(16)
O(1)-Dy(1)-O(9)	83.02(17)	O(1)-Dy(1)-N(2)	62.94(17)	O(1)-Dy(1)-N(4)	67.91(17)
O(1)-Dy(1)-N(6)	135.15(18	O(18)-Dy(2)-O(13)	81.40(16)	O(18)-Dy(2)-O(14)	81.72(15)
O(18)-Dy(2)-O(17)	129.64(16	O(18)-Dy(2)-O(21)2	142.58(16)	O(2)-Dy(1)-O(1)	130.67(16
O(18)-Dy(2)-O(22)	80.73(15)	O(2)-Dy(1)-O(5)	141.55(17)	O(18)-Dy(2)-N(8)	74.09(17)
O(2)-Dy(1)-O(6)	80.73(17)	O(18)-Dy(2)-N(10)	67.61(18)	O(2)-Dy(1)-O(9)	82.49(17)
O(18)-Dy(2)-N(12)	140.88(17	O(2)-Dy(1)-N(2)	67.96(17)	O(2)-Dy(1)-N(4)	141.42(18
O(2)-Dy(1)-N(6)	74.34(18)	O(21)2-Dy(2)-N(8)	68.58(17)	O(21)2-Dy(2)-N(10)	135.56(18
O(21)2-Dy(2)-N(12	62.42(17)	O(5)-Dy(1)-N(2)	135.37(18)	O(5)-Dy(1)-N(4)	61.91(18)

O(5)-Dy(1)-N(6)	67.37(18)	O(6) -Dy(1)-Na(1)	37.08(12)	O(22)2-Dy(2)-O(13)	141.21(15
O(22)2-Dy(2)-O(17	80.96(15)	O(22)2-Dy(2)-O(21)2	129.09(15)	O(6-Dy(1)-O(1)	82.16(17)
O(22)2-Dy(2)-N(8)	141.71(16	O(6)-Dy(1)-O(5)	129.68(17)	O(22)2-Dy(2)-N(10)	73.59(16)
O(6)-Dy(1)-O(9)	141.51(17	O(22)2-Dy(2)-N(12)2	66.74(16)	O(6)-Dy(1)-N(2)	74.53(18)
O(6)-Dy(1)-N(4)	67.85(18)	O(6)-Dy(1)-N(6)	142.67(18)	O(9)-Dy(1)-O(5)	82.71(17)
O(9)-Dy(1)-N(2)	67.09(18)	O(9)-Dy(1)-N(4)	136.09(18)	O(9)-Dy(1)-N(6)	61.88(18)
O(10)-Dy(1)-O(2)	79.59(17)	O(10)-Dy(1)-O(5)	83.31(17)	O(10)-Dy(1)-O(6)	80.10(16)
O(10-Dy(1)-O(9)	130.11(17	O(10)-Dy(1)-N(2)	141.30(18)	O(14)2-Na(2)-Dy(2)	111.75(14
O(10)-Dy(1)-N(4)	73.61(18)	O(10)-Dy(1)-N(6)	68.51(17)	N(2)-Dy(1)-N(4)	120.76(19
N(2)-Dy(1)-N(6)	119.03(18	O(14)2-Na(2)-O(14)	133.1(2)	O(14)2-Na(2)-O(15)	71.03(14)
O(14)-Na(2)-O(15)	148.48(17	O(14)2-Na(2)-O(15)	148.48(17)	O(14)-Na(2)-O(15)	71.03(14)
O(14)-Na(2)-O(22)	80.78(15)	N(6)-Dy(1)-N(4)	118.77(19)	O(14)-Na(2)-O(22)2	76.21(14)
O(14)2-Na(2)-O(22	80.78(15)	O(14)2-Na(2)-O(22)	76.21(14)	O(15)2-Na(2)-O(15)	97.0(2)
O(15)-Na(2)-O(22)	91.46(14)	O(15)-Na(2)-O(22)2	129.67(15)	O(15)2-Na(2)-O(22)	91.47(14)
O(6)-Na(1)-O(2)	75.46(16)	O(15)2-Na(2)-O(22)	129.67(15)	O(6)1-Na(1)-O(2)	120.80(17
O(6)-Na(1)-O(6)1	80.75(19)	O(6)-Na(1)-O(7)	69.61(18)	O(6)-Na(1)-O(10)1	130.2(2)
O(7)-Na(1)-O(2)	125.4(2)	O(7)-Na(1)-O(6)1	93.57(19)	O(22)2-Na(2)-O(22)	119.9(2)
O(10)-1Na(1)-O(2)	80.32(17)	O(10)1-Na(1)O(6)1	75.45(17)	O(10)1-Na(1)-O(7)	153.4(2)
O(10)1-Na(1)-O(11)	69.79(18)	O(11)1-Na(1)-O(2)	93.11(18)	O(11)1-Na(1)-O(6)1	125.7(2)
O(11)1-Na(1)-O(7)	99.3(2)	O(2)1-Na(4)-O(2)	131.1(3)	O(2)1-Na(4)-O(3)1	70.54(17)
O(2)-Na(4)-O(3)	70.54(17)	O(2) -Na(4)-O(3)1	150.92(19)	O(2)1-Na(4)-O(3)	150.92(19
O(2)1-Na(4)-O(10)	74.77(16)	O(2)-Na(4)-O(10)	74.78(16)	O(18)-Na(3)-O(14)	75.46(15)
O(2)-Na(4)-O(10)1	81.53(17)	O(18)2-Na(3)-O(14)	120.10(16)	O(2)1-Na(4)-O(10)	81.52(17)
O(18)-Na(3)-O(18)	81.70(19)	O(18)-Na(3)-O(19)	70.97(17)	O(18)-Na(3)-O(23)	149.7(2)
O(19)-Na(3)-O(14)	129.59(19	O(19)-Na(3)-O(18)2	91.07(17)	O(3)-Na(4)-O(3)1	98.4(3)
O(19)-Na(3)-O(23)	97.32(19)	O(3)-Na(4)-O(10)1	92.80(17)	O(3)1-Na(4)-O(10)1	126.75(17
O(3)-Na(4)-O(10)	126.75(17	O(3)1-Na(4)-O(10)	92.80(17)	O(22)-Na(3)-Dy(2)	110.75(13
O(22-Na(3)-O(18)	132.12(19	O(22)-Na(3)-O(18)2	75.70(15)	O(22)-Na(3)-O(19)	149.3(2)
O(22)-Na(3)-O(23)	71.02(17)	O(23)-Na(3)-O(14)	93.19(17)	O(23)-Na(3)-O(18)2	127.3(2)
O(13)-Dy(2)-O(21)	83.69(16)	O(13)-Dy(2)-N(8)	62.48(16)	O(13)-Dy(2)-N(10)	67.81(17)
O(13)-Dy(2)-N(12)	137.71(17	O(14)-Dy(2)-O(13)	129.41(15)	O(14)-Dy(2)-O(17)	140.14(14
O(14)-Dy(2)-O(21)	81.70(15)	O(14)-Dy(2)-O(22)2	81.28(15)	O(14)-Dy(2)-N(8)	67.07(15)
O(14)-Dy(2)-N(10)	142.75(17	O(14)-Dy(2)-N(12)2	72.69(16)		

Complex **2a**							
Dy(2)-O(17)	2.304(10)	Dy(4)-O(8)	2.324(10)	Dy(1)-O(20)	2.403(9)	Dy(3)-O(15)	2.384(10)
Dy(2)-O(20)	2.318(10)	Dy(4)-O(9)	2.438(10)	Dy(1)-O(24)	2.402(10)	Dy(3)-O(8)	2.362(10)
Dy(2)-O(14)	2.393(10)	Dy(4)-O(11)	2.359(10)	Dy(1)-O(3)	2.403(9)	Dy(3)-O(17)	2.398(10)
Dy(2)-O(1)	2.481(9)	Dy(4)-O(1)	2.515(9)	Dy(1)-O(1)	2.545(9)	Dy(3)-O(11)	2.325(9)
Dy(2)-N(13)	2.598(12)	Dy(4)-O(5)	2.310(9)	Dy(1)-O(5)	2.385(9)	Dy(3)-O(14)	2.321(9)
Dy(2)-O(23)	2.403(10)	Dy(4)-O(2)	2.428(10)	Dy(1)-N(15)	2.644(11)	Dy(3)-O(1)	2.521(9)
Dy(2)-O(18)	2.416(10)	Dy(4)-O(6)	2.395(10)	Dy(1)-N(1)	2.647(11)	Dy(3)-O(12)	2.459(10)
Dy(2)-O(21)	2.408(11)	Dy(4)-N(4)	2.601(10)	Dy(1)-O(23)	2.316(10)	Dy(3)-N(9)	2.676(11)
Dy(2)-N(11)	2.633(12)	Dy(4)-N(5)	2.606(12)	Dy(1)-O(2)	2.301(10)	Dy(3)-N(7)	2.630(12)

O(17)-Dy(2)-O(20)	138.3(3)	O(20)-Dy(2)-O(21)	125.6(3)	O(23)-Dy(2)-O(18)	144.1(3)
O(17)-Dy(2)-O(14)	77.5(3)	O(20)-Dy(2)-N(11)	148.1(4)	O(23)-Dy(2)-O(21)	75.2(3)
O(17)-Dy(2)-O(1)	68.8(3)	O(14)-Dy(2)-O(1)	66.5(3)	O(23)-Dy(2)-N(11)	133.7(4)
O(17)-Dy(2)-N(13)	146.0(4)	O(14)-Dy(2)-N(13)	133.4(4)	O(18)-Dy(2)-O(1)	134.3(3)
O(17)-Dy(2)-O(23)	87.5(3)	O(14)-Dy(2)-O(23)	133.7(3)	O(18)-Dy(2)-N(13)	65.7(4)
O(17)-Dy(2)-O(18)	125.0(3)	O(14)-Dy(2)-O(18)	74.4(3)	O(18)-Dy(2)-N(11)	62.1(4)
O(17)-Dy(2)-O(21)	84.1(3)	O(14)-Dy(2)-O(21)	143.9(3)	O(21)-Dy(2)-O(1)	133.7(3)
O(17)-Dy(2)-N(11)	67.0(4)	O(14)-Dy(2)-N(11)	79.6(3)	O(21)-Dy(2)-N(13)	62.5(4)
O(20)-Dy(2)-O(14)	87.4(3)	O(1)-Dy(2)-N(13)	130.4(3)	O(21)-Dy(2)-O(18)	91.9(3)
O(20)-Dy(2)-O(1)	69.6(3)	O(1)-Dy(2)-N(11)	128.6(3)	O(21)-Dy(2)-N(11)	64.6(4)
O(20)-Dy(2)-N(13)	67.6(4)	N(13)-Dy(2)-N(11)	101.0(4)	O(8)Dy(4)-O(9)	124.7(3)
O(20)-Dy(2)-O(23)	75.2(4)	O(23)-Dy(2)-O(1)	67.2(3)	O(8)-Dy(4)O(11)	76.6(4)
O(20)-Dy(2)-O(18)	86.4(3)	O(23)-Dy(2)-N(13)	78.7(3)	O(8)-Dy(4)-O(1)	67.9(3)
O(8)-Dy(4)-O(2)	86.3(3)	O(11)-Dy(4)-N(5)	78.6(4)	O(2)-Dy(4)-O(1)	66.4(3)
O(8)-Dy(4)-O(6)	86.5(4)	O(1)-Dy(4)-N(4)	131.2(3)	O(2)-Dy(4)-N(4)	82.5(3)
O(8)-Dy(4)-N(4)	149.1(4)	O(1)-Dy(4)-N(5)	127.2(3)	O(2)-Dy(4)-N(5)	133.2(4)
O(8)-Dy(4)-N(5)	66.3(4)	O(5)-Dy(4)-O(8)	137.2(3)	O(6)-Dy(4)-O(9)	91.2(4)
O(9)-Dy(4)-O(1)	134.2(3)	O(5)-Dy(4)-O(9)	86.7(3)	O(6)-Dy(4)-O(1)	134.6(3)
O(9)-Dy(4)-N(4)	63.6(3)	O(5)-Dy(4)-O(11)	87.3(3)	O(6)-Dy(4)-O(2)	75.5(4)
O(9)-Dy(4)-N(5)	62.6(4)	O(5)-Dy(4)-O(1)	69.4(3)	O(6)-Dy(4)-N(4)	62.8(4)
O(11)-Dy(4)-O(9)	74.1(3)	O(5)-Dy(4)-O(2)	76.1(3)	O(6)-Dy(4)-N(5)	66.1(4)
O(11)-Dy(4)-O(1)	66.5(3)	O(5)-Dy(4)-O(6)	124.6(3)	N(4)-Dy(4)-N(5)	101.6(4)
O(11)-Dy(4)-O(2)	132.9(3)	O(5)-Dy(4)-N(4)	67.1(3)	O(20)-Dy(1)-O(1)	67.2(3)
O(11)-Dy(4)-O(6)	144.5(4)	O(5)-Dy(4)-N(5)	148.7(4)	O(20)-Dy(1)-N(15)	77.6(3)
O(11)-Dy(4)-N(4)	130.9(3)	O(2)-Dy(4)-O(9)	145.9(3)	O(20)-Dy(1)-N(1)	132.8(4)
O(24)-Dy(1)-O(20)	77.4(3)	O(5)-Dy(1)-O(24)	142.3(3)	O(23)-Dy(1)-N(1)	150.1(4)
O(24)-Dy(1)-O(3)	86.0(3)	O(5)-Dy(1)-O(3)	75.5(3)	O(2)-Dy(1)-Dy(2)	101.3(2)
O(24)-Dy(1)-O(1)	137.1(3)	O(5)-Dy(1)-O(1)	67.7(3)	O(2)-Dy(1)-Dy(4)	42.6(2)
O(24)-Dy(1)-N(15)	62.4(4)	O(5)-Dy(1)-N(15)	132.1(4)	O(2)-Dy(1)-O(20)	87.4(3)
O(24)-Dy(1)-N(1)	63.8(3)	O(5)-Dy(1)-N(1)	78.6(3)	O(2)-Dy(1)-O(24)	87.9(3)
O(3)-Dy(1)-O(20)	142.8(3)	N(15)-Dy(1)-N(1)	104.7(3)	O(2)-Dy(1)-O(3)	125.4(3)
O(3)-Dy(1)-O(1)	136.9(3)	O(23)-Dy(1)-O(20)	75.2(3)	O(2)-Dy(1)-O(1)	67.7(3)
O(3)-Dy(1)-N(15)	65.3(3)	O(23)-Dy(1)-O(24)	126.4(3)	O(2)-Dy(1)-O(5)	77.2(3)
O(1)-Dy(1)-N(15)	127.8(3)	O(23)-Dy(1)-O(1)	67.4(3)	O(15)-Dy(3)-O(17)	74.7(3)
O(1)-Dy(1)-N(1)	127.6(3)	O(23)-Dy(1)-O(5)	86.4(3)	O(15)-Dy(3)-O(1)	136.1(3)
O(5)-Dy(1)-O(20)	134.9(3)	O(23)-Dy(1)-N(15)	67.2(3)	O(15)-Dy(3)-O(12)	86.6(4)
O(15)-Dy(3)-N(9)	63.0(3)	O(11)-Dy(3)-O(15)	90.1(3)	O(14)-Dy(3)-O(12)	91.5(4)
O(15)-Dy(3)-N(7)	63.7(4)	O(11)-Dy(3)-O(8)	76.5(4)	O(14)-Dy(3)-N(9)	66.4(3)
O(8)-Dy(3)-O(15)	145.4(3)	O(11)-Dy(3)-O(17)	84.8(3)	O(14)-Dy(3)-N(7)	153.6(4)
O(8)-Dy(3)-O(17)	133.9(3)	O(11)-Dy(3)-O(1)	66.9(3)	O(1)-Dy(3)-N(9)	128.4(3)
O(8)-Dy(3)-O(1)	67.2(3)	O(11)-Dy(3)-O(12)	123.6(3)	O(1)-Dy(3)-N(7)	127.7(3)
O(8)-Dy(3)-O(12)	75.3(4)	O(11)-Dy(3)-N(9)	152.5(4)	O(12)-Dy(3)-O(1)	137.3(4)
O(8)-Dy(3)-N(9)	128.8(4)	O(11)-Dy(3)-N(7)	65.5(4)	O(12)-Dy(3)-N(9)	63.9(4)
O(8)-Dy(3)-N(7)	81.8(4)	O(14)-Dy(3)-O(15)	124.1(3)	O(12)-Dy(3)-N(7)	62.8(4)

O(17)-Dy(3)-O(1)	66.7(3)	O(14)-Dy(3)-O(8)	86.2(3)	N(7)-Dy(3)-N(9)	103.9(4)
O(17)-Dy(3)-O(12)	146.4(3)	O(14)-Dy(3)-O(17)	77.1(3)	O(3)-Dy(1)-N(1)	62.3(3)
O(17)-Dy(3)-N(9)	82.7(3)	O(14)-Dy(3)-O(11)	133.7(3)	O(23)-Dy(1)-O(3)	89.0(3)
O(17)-Dy(3)-N(7)	127.5(4)	O(14)-Dy(3)-O(1)	66.9(3)	O(2)-Dy(1)-N(15)	148.8(4)

Complex **2b**							
Dy(1)-O(1)	2.540(4)	Dy(2)-O(1)	2.492(4)	Dy(3)-O(1)	2.544(4)	Dy(4)-O(1)	2.496(4)
Dy(1)-O(2)	2.303(4)	Dy(2)-O(2)	2.402(4)	Dy(3)-O(8)	2.311(4)	Dy(4)-O(11)	2.328(4)
Dy(1)-O(3)	2.407(4)	Dy(2)-O(5)	2.317(4)	Dy(3)-O(9)	2.392(4)	Dy(4)-O(12)	2.425(4)
Dy(1)-O(5)	2.399(4)	Dy(2)-O(6)	2.391(4)	Dy(3)-O(11)	2.373(4)	Dy(4)-O(15)	2.310(4)
Dy(1)-O(12)	2.317(4)	Dy(2)-O(8)	2.402(4)	Dy(3)-O(18)	2.313(4)	Dy(4)-O(16)	2.398(5)
Dy(1)-O(13)	2.397(4)	Dy(2)-O(9)	2.301(4)	Dy(3)-O(19)	2.453(5)	Dy(4)-O(18)	2.373(4)
Dy(1)-O(15)	2.373(4)	Dy(2)-N(3)	2.619(5)	Dy(3)-O(23)	2.387(4)	Dy(4)-O(21)	2.429(4)
Dy(1)-N(1)	2.644(5)	Dy(2)-O(37)	2.430(4)	Dy(3)-N(11)	2.621(5)	Dy(4)-N(9)	2.642(5)
Dy(1)-N(7)	2.665(5)	Dy(2)-N(20)	2.631(5)	Dy(3)-N(16)	2.640(5)	Dy(4)-N(14)	2.617(5)

O(1)-Dy(1)-N(1)	128.03(14)	O(6)-Dy(2)-O(1)	133.81(15)	O(18)-Dy(3)-N(16)	152.03(16)
O(1)-Dy(1)-N(7)	127.04(13)	O(6)-Dy(2)-O(2)	76.12(15)	O(19)-Dy(3)-O(1)	138.02(16)
O(2)-Dy(1)-O(1)	67.16(14)	O(6)-Dy(2)-O(8)	143.01(14)	O(19)-Dy(3)-N(11)	61.82(17)
O(2)-Dy(1)O(3)	126.03(14)	O(6)-Dy(2)-N(3)	62.59(16)	O(19)-Dy(3)-N(16)	64.45(16)
O(2)-Dy(1)-O(5)	75.01(15)	O(6)-Dy(2)-O(37)	92.15(15)	O(23)-Dy(3)-O(1)	136.21(15)
O(2)-Dy(1)-O(12)	134.28(14)	O(6)-Dy(2)-N(20)	64.47(16)	O(23)-Dy(3)-O(9)	74.76(14)
O(2)-Dy(1)-O(13)	90.09(15)	O(8)-Dy(2)-O(1)	66.50(13)	O(18)-Dy(3)-N(16)	152.03(16)
O(2)-Dy(1)-O(15)	86.42(14)	O(8)-Dy(2)-O(2)	133.03(13)	O(19)-Dy(3)-O(1)	138.02(16)
O(2)-Dy(1)-N(1)	67.01(14)	O(8)-Dy(2)-N(3)	134.89(15)	O(19)-Dy(3)-N(11)	61.82(17)
O(2)-Dy(1)-N(7)	150.86(16)	O(8)-Dy(2)-O(37)	75.12(14)	O(19)-Dy(3)-N(16)	64.45(16)
O(1)-Dy(1)-N(1)	128.03(14)	O(8)-Dy(2)-N(20)	79.03(15)	O(1)-Dy(4)-N(9)	130.45(14)
O(3)-Dy(1)-O(1)	137.42(14)	O(9)-Dy(2)-O(1)	69.28(14)	O(1)-Dy(4)-N(14)	128.31(14)
O(3)-Dy(1)N(1)	62.53(15)	O(9)-Dy(2)-O(2)	87.75(14)	O(11)-Dy(4)-O(1)	68.68(14)
O(3)-Dy(1)-N(7)	64.01(15)	O(9)-Dy(2)-O(5)	138.36(14)	O(11)-Dy(4)-O(12)	86.73(14)
O(5)-Dy(1)-O(1)	67.06(13)	O(9)-Dy(2)-O(6)	83.49(15)	O(11)-Dy(4)-O(16)	85.66(15)
O(5)-Dy(1)-O(3)	77.57(14)	O(9)-Dy(2)-O(8)	76.87(14)	O(11)-Dy(4)-O(18)	76.61(15)
O(5)-Dy(1)-N(1)	78.62(15)	O(9)-Dy(2)-N(3)	145.38(16)	O(11)-Dy(4)-O(21)	125.01(15)
O(5)-Dy(1)-N(7)	132.51(16)	O(9)-Dy(2)-O(37)	125.72(14)	O(11)-Dy(4)-N(9)	148.08(15)
O(12)-Dy(1)-O(1)	67.12(13)	O(9)-Dy(2)-N(20)	67.31(15)	O(11)-Dy(4)-N(14)	66.86(15)
O(12)-Dy(1)-O(3)	88.77(14)	N(3)-Dy(2)-N(20)	101.10(15)	O(12)-Dy(4)-O(21)	145.12(14)
O(12)-Dy(1)-O(5)	86.99(14)	O(37)-Dy(2)-O(1)	134.02(14)	O(12)-Dy(4)-N(9)	81.35(14)
O(12)-Dy(1)-O(13)	124.85(14)	O(37)-Dy(2)-N(3)	65.98(15)	O(12)-Dy(4)-N(14)	133.92(16)
O(12)-Dy(1)-O(15)	77.05(14)	O(37)-Dy(2)-N(20)	62.33(16)	O(15)-Dy(4)-O(1)	69.40(13)
O(12)-Dy(1)-N(1)	149.94(15)	O(1)-Dy(3)-N(11)	127.17(14)	O(15)-Dy(4)-O(11)	138.07(14)
O(12)-Dy(1)-N(7)	66.31(15)	O(1)-Dy(3)-N(16)	128.40(14)	O(15)-Dy(4)-O(12)	76.14(14)
O(13)-Dy(1)-O(1)	136.94(14)	O(8)-Dy(3)-O(1)	66.93(13)	O(15)-Dy(4)-O(16)	124.84(15)
O(13)-Dy(1)-O(3)	85.61(15)	O(8)-Dy(3)-O(9)	76.88(14)	O(15)-Dy(4)-O(18)	87.45(14)
O(13)-Dy(1)-O(5)	143.78(14)	O(8)-Dy(3)-O(11)	86.17(14)	O(15)-Dy(4)-O(21)	85.95(15)

O(13)-Dy(1)-N(1)	65.16(15)	O(8)-Dy(3)-O(18)	133.48(14)	O(15)-Dy(4)-N(9)	66.97(15)
O(13)-Dy(1)-N(7)	62.07(16)	O(37)-Dy(2)-O(1)	134.02(14)	O(15)-Dy(4)-N(14)	147.49(17)
O(15)-Dy(1)-O(1)	67.70(13)	O(8)-Dy(3)-O(23)	124.42(14)	O(16)-Dy(4)-O(1)	134.32(15)
O(15)-Dy(1)-O(3)	142.55(15)	O(8)-Dy(3)-N(11)	153.51(17)	O(16)-Dy(4)-O(12)	75.43(14)
O(15)-Dy(1)-O(5)	134.73(14)	O(8)-Dy(3)-N(16)	66.47(15)	O(16)-Dy(4)-O(21)	91.50(15)
O(15)-Dy(1)-O(13)	75.14(14)	O(9)-Dy(3)-O(1)	67.06(13)	O(16)-Dy(4)-N(9)	62.73(16)
O(15)-Dy(1)-N(1)	131.10(15)	O(9)-Dy(3)O(19)	146.13(14)	O(16)-Dy(4)-N(14)	65.93(16)
O(15)-Dy(1)-N(7)	78.57(15)	O(9)-Dy(3)-N(11)	127.96(17)	O(18)-Dy(4)-O(1)	66.53(13)
N(1)-Dy(1)-N(7)	104.93(15)	O(9)-Dy(3)-N(16)	81.94(15)	O(18)-Dy(4)-O(12)	132.83(13)
O(1)-Dy(2)-N(3)	129.68(14)	O(11)-Dy(3)-O(1)	67.19(14)	O(18)-Dy(4)-O(16)	144.36(15)
O(2)-Dy(2)-O(1)	66.54(13)	O(11)-Dy(3)-O(9)	134.24(14)	O(18)-Dy(4)-O(21)	74.65(14)
O(2)-Dy(2)-N(3)	78.06(14)	O(11)-Dy(3)-O(19)	75.59(15)	O(18)-Dy(4)-N(9)	131.96(15)
O(2)-Dy(2)-O(37)	143.48(13)	O(11)-Dy(3)-O(23)	145.12(14)	O(18)-Dy(4)-N(14)	78.66(16)
O(2)-Dy(2)-N(20)	134.77(16)	O(11)-Dy(3)-N(11)	81.15(16)	O(21)-Dy(4)-O(1)	134.18(15)
O(5)-Dy(2)-O(1)	69.10(13)	O(11)-Dy(3)-N(16)	129.15(16)	O(21)-Dy(4)-N(9)	64.04(15)
O(5)-Dy(2)-O(2)	74.71(15)	O(18)-Dy(3)-O(1)	66.56(13)	O(21)-Dy(4)-N(14)	62.15(17)
O(5)-Dy(2)-O(6)	126.24(15)	O(18)-Dy(3)-O(9)	84.64(14)	N(14)-Dy(4)-N(9)	101.22(15)
O(5)-Dy(2)-O(8)	87.94(14)	O(18)-Dy(3)-O(11)	76.88(15)	O(18)-Dy(4)N(9)	131.96(15)
O(5)-Dy(2)-N(3)	67.79(15)	O(18)-Dy(3)-O(19)	123.36(15)	O(5)-Dy(2)-N(20)	147.51(16)
O(5)-Dy(2)-O(37)	85.66(14)	O(18)-Dy(3)-O(23)	89.85(15)	O(18)-Dy(3)-N(11)	65.71(16)

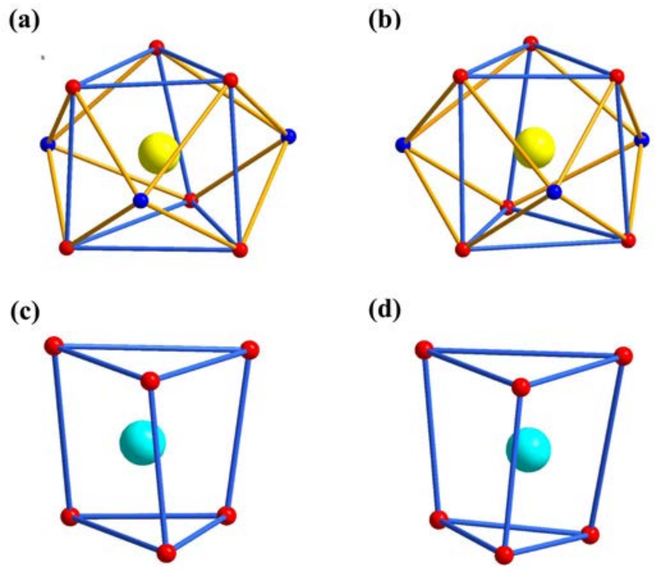


Figure S5 Coordination geometry of Dy^{3+} ions in (a) complex **1a** and (b) complex **1b**. (Dy^{3+}: yellow, O : red, N : blue) Coordination geometry of Na^{+} ions in (c) complex **1a** and (d) complex **1b**. (O : red, N : blue, Na^{+}: light blue)

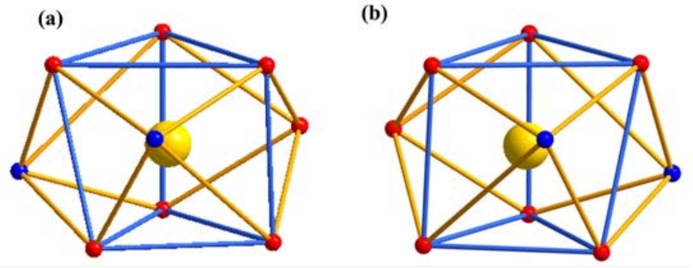


Figure S6 Coordination geometry of Dy^{3+} ions in (a) complex **2a** and (b) complex **2b.** (Dy^{3+}: yellow, O : red, N : blue)

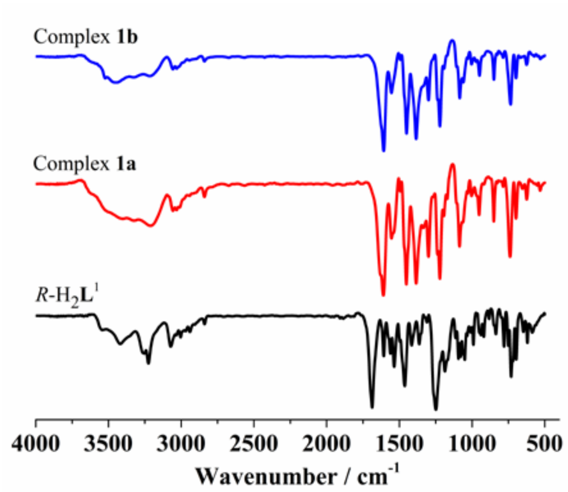


Figure S7 IR spectra of complex **1a**, complex **1b** and *S*-H_2**L**^{1}.

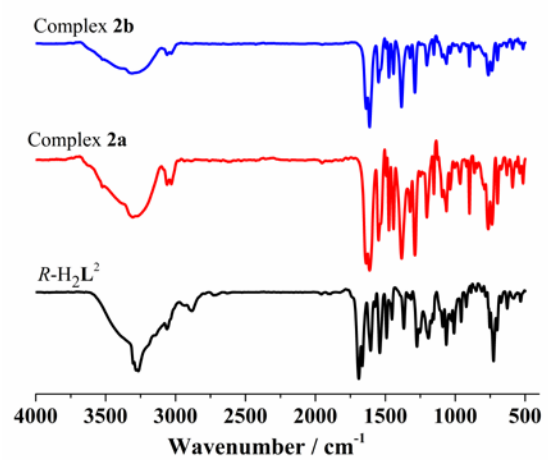


Figure S8 IR spectra of complex **2a**, complex **2b** and *S*-H_2**L**^{2}.

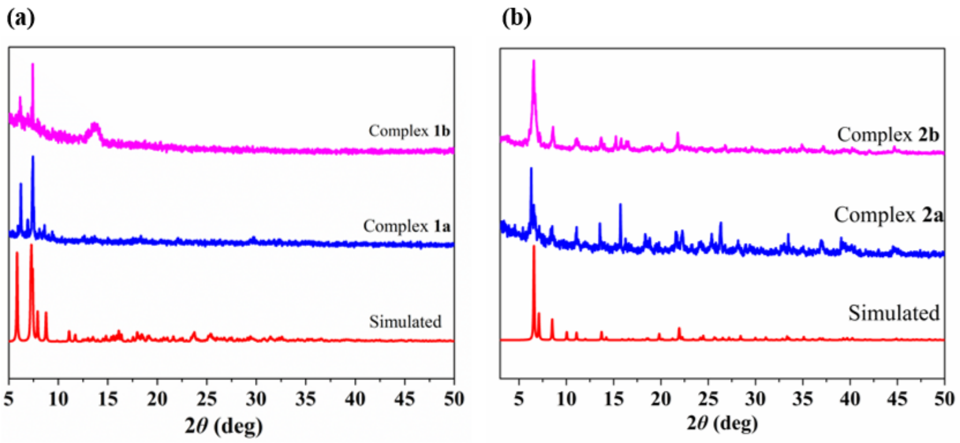


Figure S9 Comparing the simulated PXRD with experimental patterns.

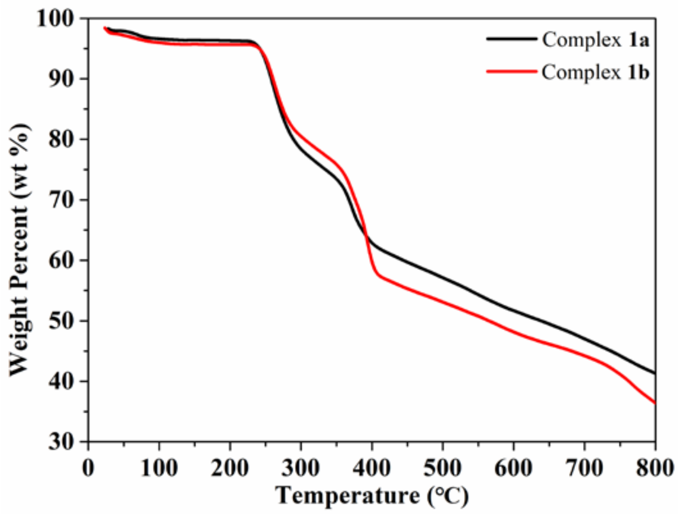


Figure S10 TGA spectra of complex **1a** and **1b.**

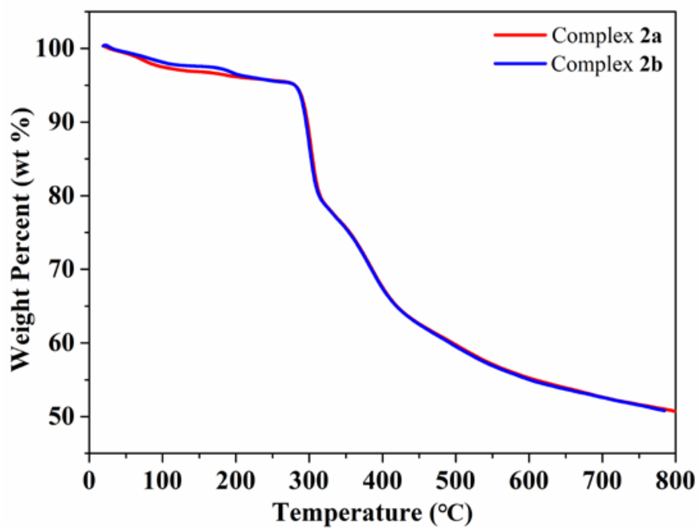


Figure S11 TGA spectra of complex **2a** and **2b.**

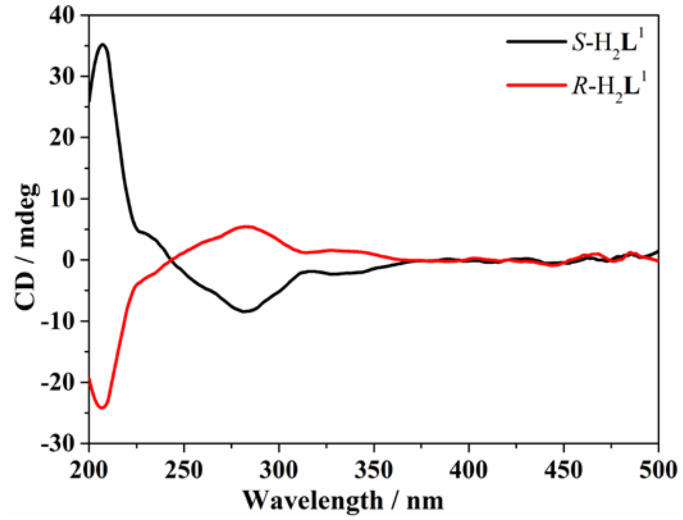


Figure S12 CD spectra of *S*-H_2**L**^{1} and *R*-H_2**L**^{1} in methanol solution (3 ×10^{-4} M).

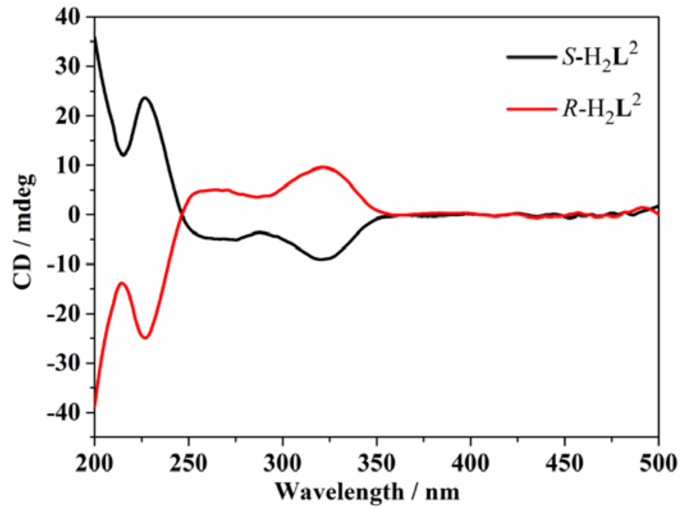


Figure S13 CD spectra of *S*-H_2**L**^{2} and *R*-H_2**L**^{2} in methanol solution (3 ×10^{-4} M).

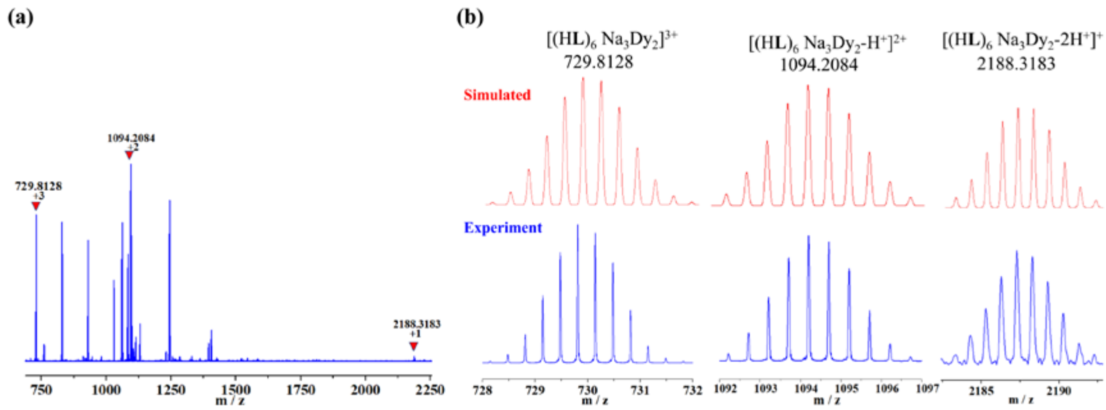


Figure S14 (a) HRESI-MS spectrum of complex **1a** in methanol. (b) Compared the experimental isotopic distribution with the theoretical isotopic distribution and the assignments of corresponding peaks.

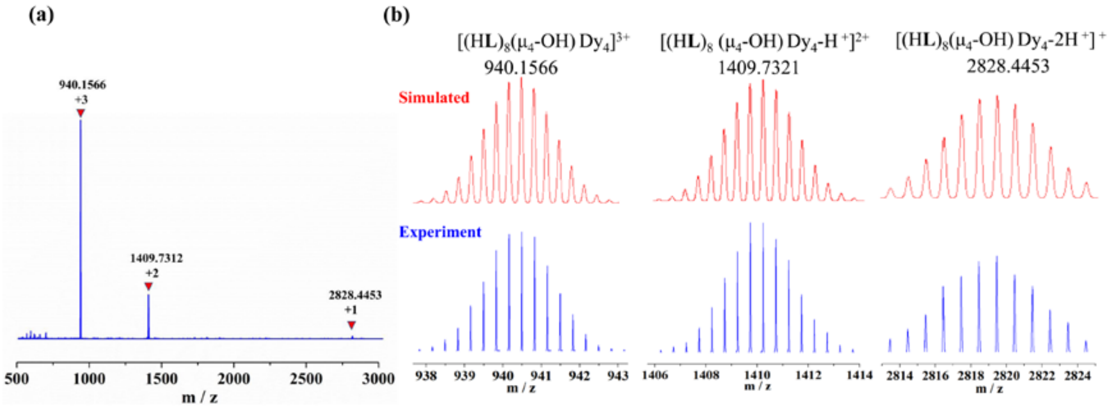


Figure S15 (a) HRESI-MS spectrum of complex **2a** in methanol. (b) Compared the experimental isotopic distribution with the theoretical isotopic distribution and the assignments of corresponding peaks.

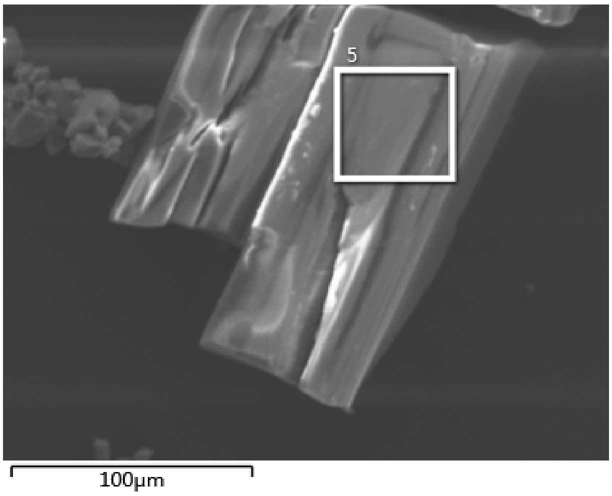


Figure S16 SEM image of crystal prepared from mixed-metal experiment.

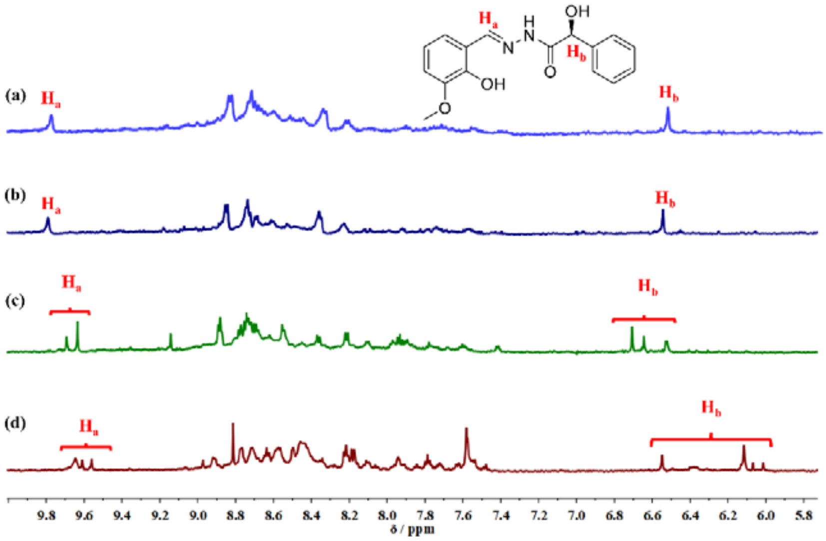


Figure S17. The partial ^{1}H-NMR spectra (CD_3OD and CD_3CN; v:v = 2:1) of (*S*)-H_2**L**^{1} with the mixed metal ions and single metal ions: (a) mixed metal ions; (b) Na^+; (c) K^+; (d) Li^+.