Seven Dicarboxylate-Based Coordination Polymers with Structural Varieties and Solvent Resistance Property Changing Derived from the Introduction of Small Organic Linkers

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Table S1. Selected Bond Lengths (Å) and Bond Angles (deg) for **1**–**7**

Compound **1**			
Co(1)-O(7)	2.054(5)	Co(2)-O(17)	2.056(6)
Co(1)-O(2)	2.062(5)	Co(2)-O(1)	2.075(6)
Co(1)-O(14)	2.063(5)	Co(2)-O(2)	2.280(5)
Co(1)-O(5)#1	2.092(5)	Co(2)-O(16)	2.294(12)
Co(1)-O(13)#2	2.109(6)	Co(3)-O(12)#2	1.938(5)
Co(1)-O(21)#3	2.127(6)	Co(3)-O(20)#3	1.956(6)
Co(2)-O(6)#1	1.997(5)	Co(3)-O(8)	1.971(5)
Co(2)-O(15)	2.032(6)	Co(3)-O(9)	2.149(11)
O(7)-Co(1)-O(2)	176.2(3)	O(6)#1-Co(2)-O(1)	153.5(2)
O(7)-Co(1)-O(14)	85.7(2)	O(15)-Co(2)-O(1)	97.5(3)
O(2)-Co(1)-O(14)	97.7(2)	O(17)-Co(2)-O(1)	101.8(3)
O(7)-Co(1)-O(5)#1	89.5(2)	O(6)#1-Co(2)-O(2)	95.8(2)
O(2)-Co(1)-O(5)#1	88.6(2)	O(15)-Co(2)-O(2)	99.4(2)
O(14)-Co(1)-O(5)#1	94.1(2)	O(17)-Co(2)-O(2)	159.3(2)
O(7)-Co(1)-O(13)#2	95.4(2)	O(1)-Co(2)-O(2)	59.2(2)
O(2)-Co(1)-O(13)#2	86.5(2)	O(6)#1-Co(2)-O(16)	82.6(3)
O(14)-Co(1)-O(13)#2	86.0(2)	O(15)-Co(2)-O(16)	176.9(3)
O(5)#1-Co(1)-O(13)#2	175.1(2)	O(17)-Co(2)-O(16)	87.6(3)
O(7)-Co(1)-O(21)#3	86.5(2)	O(1)-Co(2)-O(16)	85.4(3)
O(2)-Co(1)-O(21)#3	90.2(2)	O(2)-Co(2)-O(16)	82.9(3)
O(14)-Co(1)-O(21)#3	171.3(2)	O(12)#2-Co(3)-O(20)#3	124.6(3)
O(5)#1-Co(1)-O(21)#3	89.8(2)	O(12)#2-Co(3)-O(8)	113.3(3)
O(13)#2-Co(1)-O(21)#3	90.8(2)	O(20)#3-Co(3)-O(8)	114.6(3)
O(6)#1-Co(2)-O(15)	95.2(3)	O(12)#2-Co(3)-O(9)	98.1(3)
O(6)#1-Co(2)-O(17)	101.2(2)	O(20)#3-Co(3)-O(9)	98.6(4)
O(15)-Co(2)-O(17)	90.8(2)	O(8)-Co(3)-O(9)	100.9(3)
Symmetry codes: #1 = -x+1, y+1/2, -z+1/2; #2 = -x+2, y-1/2, -z+1/2; #3 = x-1, -y+3/2, z-1/2.			
Compound **2**			
Co(1)-O(1)#1	2.010(2)	Co(2)-O(1)	2.074(2)
Co(1)-O(8)#2	2.013(3)	Co(2)-N(2)	2.083(3)
Co(1)-N(3)	2.018(3)	Co(2)-N(1)#3	2.089(3)
Co(1)-O(4)#1	2.068(2)	Co(2)-O(7)#4	2.195(3)
Co(1)-O(1)	2.167(2)	Co(2)-O(2)	2.196(3)
Co(2)-O(3)	2.069(2)	O(1)-Co(2)-N(2)	88.14(9)
O(1)#1-Co(1)-O(8)#2	125.56(10)	O(3)-Co(2)-N(1)#3	87.10(10)
O(1)#1-Co(1)-N(3)	115.80(10)	O(1)-Co(2)-N(1)#3	176.60(10)
O(8)#2-Co(1)-N(3)	116.40(11)	N(2)-Co(2)-N(1)#3	94.28(10)
O(1)#1-Co(1)-O(4)#1	98.65(9)	O(3)-Co(2)-O(7)#4	88.06(10)
O(8)#2-Co(1)-O(4)#1	94.05(10)	O(1)-Co(2)-O(7)#4	95.76(10)

N(3)-Co(1)-O(4)#1	91.88(10)	N(2)-Co(2)-O(7)#4	89.47(11)
O(1)#1-Co(1)-O(1)	79.19(9)	N(1)#3-Co(2)-O(7)#4	86.66(11)
O(8)#2-Co(1)-O(1)	89.00(10)	O(3)-Co(2)-O(2)	87.25(10)
N(3)-Co(1)-O(1)	87.14(9)	O(1)-Co(2)-O(2)	90.57(10)
O(4)#1-Co(1)-O(1)	176.92(9)	N(2)-Co(2)-O(2)	95.38(10)
O(3)-Co(2)-O(1)	90.59(9)	N(1)#3-Co(2)-O(2)	86.83(11)
O(3)-Co(2)-N(2)	177.09(10)	O(7)#4-Co(2)-O(2)	172.16(10)
Symmetry codes: #1 = -x+2, -y+1, -z; #2 = x+1/2, y, -z+1/2; #3 = y+1/4, -x+7/4, -z-1/4; #4 = -x+3/2, -y+1, z-1/2.			
Compound **3**			
Co(1)-N(3)	2.079(8)	Co(2)-O(1)#1	2.002(8)
Co(1)-N(2)	2.080(7)	Co(2)-O(7)	2.017(6)
Co(1)-O(5)	2.080(7)	Co(2)-N(1)#2	2.017(7)
Co(1)-O(7)	2.100(6)	Co(2)-O(6)	2.079(7)
Co(1)-O(2)#1	2.161(8)	Co(2)-O(7)#2	2.177(6)
Co(1)-O(8)	2.220(8)	O(5)-Co(1)-O(8)	86.9(3)
N(3)-Co(1)-N(2)	98.3(3)	O(7)-Co(1)-O(8)	86.9(3)
N(3)-Co(1)-O(5)	85.7(3)	O(2)#1-Co(1)-O(8)	171.5(3)
N(2)-Co(1)-O(5)	173.8(3)	O(1)#1-Co(2)-O(7)	121.9(3)
N(3)-Co(1)-O(7)	171.4(3)	O(1)#1-Co(2)-N(1)#2	121.7(3)
N(2)-Co(1)-O(7)	88.0(3)	O(7)-Co(2)-N(1)#2	114.4(3)
O(5)-Co(1)-O(7)	88.6(3)	O(1)#1-Co(2)-O(6)	93.2(3)
N(3)-Co(1)-O(2)#1	87.1(3)	O(7)-Co(2)-O(6)	98.8(3)
N(2)-Co(1)-O(2)#1	88.1(3)	N(1)#2-Co(2)-O(6)	92.2(3)
O(5)-Co(1)-O(2)#1	87.3(3)	O(1)#1-Co(2)-O(7)#2	89.0(3)
O(7)-Co(1)-O(2)#1	99.2(3)	O(7)-Co(2)-O(7)#2	79.1(3)
N(3)-Co(1)-O(8)	86.3(3)	N(1)#2-Co(2)-O(7)#2	87.5(3)
N(2)-Co(1)-O(8)	98.1(3)	O(6)-Co(2)-O(7)#2	177.6(3)
Symmetry codes: #1 = -x+1/2, -y, z-1/2; #2 = -x+1, -y, -z+1.			
Compound **4**			
Co(1)-O(6)	1.988(3)	Co(1)-O(7)	2.127(4)
Co(1)-N(3)	2.100(3)	Co(1)-N(1)	2.185(3)
Co(1)-O(2)#1	2.117(3)	Co(1)-O(1)#1	2.232(3)
O(6)-Co(1)-N(3)	97.89(13)	O(2)#1-Co(1)-N(1)	105.46(12)
O(6)-Co(1)-O(2)#1	157.55(12)	O(7)-Co(1)-N(1)	90.10(14)
N(3)-Co(1)-O(2)#1	92.61(12)	O(6)-Co(1)-O(1)#1	98.55(12)
O(6)-Co(1)-O(7)	92.45(16)	N(3)-Co(1)-O(1)#1	94.25(12)
N(3)-Co(1)-O(7)	165.45(15)	O(2)#1-Co(1)-O(1)#1	60.75(10)
O(2)#1-Co(1)-O(7)	81.37(15)	O(7)-Co(1)-O(1)#1	94.30(13)
O(6)-Co(1)-N(1)	96.06(13)	N(1)-Co(1)-O(1)#1	164.54(11)
N(3)-Co(1)-N(1)	78.69(13)		
Symmetry codes: #1 = -x+1, y+1, -z+1/2.			
Compound **5**			

Cu(1)-O(2)	1.960(2)	Cu(1)-O(1)#3	1.962(2)
Cu(1)-O(2)#1	1.960(2)	Cu(1)-O(4)	2.193(4)
Cu(1)-O(1)#2	1.962(2)	O(1)#2-Cu(1)-O(1)#3	88.37(15)
O(2)-Cu(1)-O(2)#1	90.22(14)	O(2)-Cu(1)-O(4)	99.66(11)
O(2)-Cu(1)-O(1)#2	168.81(10)	O(2)#1-Cu(1)-O(4)	99.66(11)
O(2)#1-Cu(1)-O(1)#2	89.62(11)	O(1)#2-Cu(1)-O(4)	91.39(11)
O(2)-Cu(1)-O(1)#3	89.62(11)	O(1)#3-Cu(1)-O(4)	91.39(11)
O(2)#1-Cu(1)-O(1)#3	168.81(10)		
Symmetry codes: #1 = x, -y+1, z; #2 = -x+1, -y+1, -z+2; #3 = -x+1, y, -z+2.			
Compound **6**			
Cu(1)-O(1)	1.952(4)	Cu(2)-O(1)#1	1.944(4)
Cu(1)-O(3)	1.971(4)	Cu(2)-O(4)	1.963(4)
Cu(1)-N(1)	1.982(5)	Cu(2)-N(3)#2	1.978(5)
Cu(1)-N(2)	1.988(5)	Cu(2)-O(7)#3	2.128(11)
Cu(1)-O(2)	2.513(9)	Cu(2)-O(1)	2.290(5)
O(1)-Cu(1)-O(3)	90.68(18)	O(1)#1-Cu(2)-O(4)	173.4(2)
O(1)-Cu(1)-N(1)	89.06(19)	O(1)#1-Cu(2)-N(3)#2	87.83(18)
O(3)-Cu(1)-N(1)	171.3(2)	O(4)-Cu(2)-N(3)#2	88.95(19)
O(1)-Cu(1)-N(2)	174.3(2)	O(1)#1-Cu(2)-O(7)#3	93.2(3)
O(3)-Cu(1)-N(2)	86.4(2)	O(4)-Cu(2)-O(7)#3	93.4(3)
N(1)-Cu(1)-N(2)	94.6(2)	N(3)#2-Cu(2)-O(7)#3	125.4(4)
O(1)-Cu(1)-O(2)	90.6(3)	O(1)#1-Cu(2)-O(1)	81.35(19)
O(3)-Cu(1)-O(2)	89.1(3)	O(4)-Cu(2)-O(1)	94.03(18)
N(1)-Cu(1)-O(2)	99.7(3)	N(3)#2-Cu(2)-O(1)	105.9(2)
N(2)-Cu(1)-O(2)	84.5(3)	O(7)#3-Cu(2)-O(1)	128.3(4)
Symmetry codes: #1 = -x+2, -y+1, -z+2; #2 = -y+5/4, x-1/4, z-1/4; #3 = -x+3/2, -y+1, z+1/2.			
Compound **7**			
Zn(1)-O(2)#1	1.955(3)	Zn(2)-O(6)	1.936(3)
Zn(1)-N(3)	1.983(4)	Zn(2)-N(4)	1.986(4)
Zn(1)-N(1)#2	2.008(4)	Zn(2)-N(8)#3	1.991(4)
Zn(1)-N(7)#3	2.022(4)	Zn(2)-N(5)	2.008(4)
O(2)#1-Zn(1)-N(3)	126.03(15)	O(6)-Zn(2)-N(4)	112.19(16)
O(2)#1-Zn(1)-N(1)#2	109.52(15)	O(6)-Zn(2)-N(8)#3	116.10(15)
N(3)-Zn(1)-N(1)#2	107.39(15)	N(4)-Zn(2)-N(8)#3	109.25(15)
O(2)#1-Zn(1)-N(7)#3	98.68(15)	O(6)-Zn(2)-N(5)	97.21(15)
N(3)-Zn(1)-N(7)#3	107.01(15)	N(4)-Zn(2)-N(5)	108.28(16)
N(1)#2-Zn(1)-N(7)#3	106.46(16)	N(8)#3-Zn(2)-N(5)	113.18(16)
Symmetry codes: #1 = x+1/2, y+1/2, -z+3/2; #2 = x, -y+2, z+1/2; #3 = -x+1/2, -y+5/2, z+1/2.			

Table S2. Hydrogen Bonds of complexes **3**, **4**, and **7**.

Complex	D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(D-H···A) (deg)
3	N(4)-H(4A) ···N(3)	0.86	2.39	3.129(12)	144.9
	N(4)-H(4B) ···O(8)	0.86	2.41	2.999(12)	125.7
4	O(7) -H(7W1) ···O(5)	0.75(6)	2.11(6)	2.836(5)	163(6)
7	N2-H(2A) ···O(1)	0.86	2.05	2.834(6)	152.0
	N6-H(6A) ···O(2)	0.86	2.24	2.984(6)	144.6
	N6-H(6B) ···O(6)	0.86	2.31	2.964(6)	133.3
	N2-H(2B) ···O(2)	0.86	2.52	3.279(6)	147.1

Table S3. Crystallographic Data and Structure Refinement Details for **1** and **5**.

Unit Cell of Parameters of complexes **1**, 5		H_2O	MeOH	EtOH	MeCN	DMF	0.5 M HCl aq.	0.5 M NaOH aq.
Complex **1**	a	-	16.61	16.60	16.62	16.60.	-	-
	b	-	20.39	20.38	20.40	20.38	-	-
	c	-	17.17	17.17	17.15	17.18	-	-
	α	-	90	90	90	90	-	-
	β	-	99.66	99.64	99.73	99.67	-	-
	γ	-	90	90	90	90	-	-
	V	-	5746	5729	5730	5732	-	-
Complex **5**	a	12.50	-	-	12.46	-	-	-
	b	22.27	-	-	22.20	-	-	-
	c	7.14	-	-	7.16	-	-	-
	α	90	-	-	90	-	-	-
	β	126.12	-	-	126.06	-	-	-
	γ	90	-	-	90	-	-	-
	V	1617	-	-	1596	-	-	-

Table S4. Crystallographic Data and Structure Refinement Details for **1** and **5**.

Unit Cell of Parameters of complexes **2-4**, **6-7**		H_2O	MeOH	EtOH	MeCN	DMF	0.5 M HCl aq.	0.5 M NaOH aq.
Complex **2**	a	25.08	25.07	25.10	25.09	25.08	-	-
	b	25.08	25.07	25.10	25.09	25.08	-	-
	c	15.03	15.02	15.04	15.01	15.02	-	-
	α	90	90	90	90	90	-	-
	β	90	90	90	90	90	-	-
	γ	90	90	90	90	90	-	-
	V	9454	9440	9475	9449	9437	-	-
Complex **3**	a	25.38	25.36	25.39	25.37	25.38		
	b	25.38	25.36	25.39	25.37	25.38		
	c	15.20	15.21	15.22	15.19	15.20		
	α	90	90	90	90	90	-	-
	β	90	90	90	90	90	-	-
	γ	90	90	90	90	90	-	-
	V	9791	9782	9811	9777	9791		
Complex **4**	a	23.44	24.49	23.46	23.46	23.44	-	-
	b	7.13	7.09	7.13	7.06	7.10		
	c	32.51	32.06	32.51	32.17	32.19		
	α	90	90	90	90	90		
	β	105.77	104.74	105.77	104.76	104.97	-	-
	γ	90	90	90	90	90	-	-
	V	5229	5163	5193	5149	5176	-	-
Complex **6**	a	24.35	24.33	24.39	24.37	24.36	-	-
	b	24.35	24.33	24.39	24.37	24.36	-	-
	c	15.07	15.10	15.08	15.06	15.09	-	-
	α	90	90	90	90	90	-	-
	β	90	90	90	90	90	-	-
	γ	90	90	90	90	90	-	-
	V	8935	8838	8970	8944	8954	-	-
Complex **7**	a	9.82	9.85	9.86	9.86	9.84	-	-
	b	16.54	16.56	16.59	16.59	16.52	-	-
	c	30.55	30.63	30.67	30.66	30.59	-	-
	α	90	90	90	90	90	-	-
	β	90	90	90	90	90	-	-
	γ	90	90	90	90	90	-	-
	V	4959	4998	5018	5017	4974	-	-

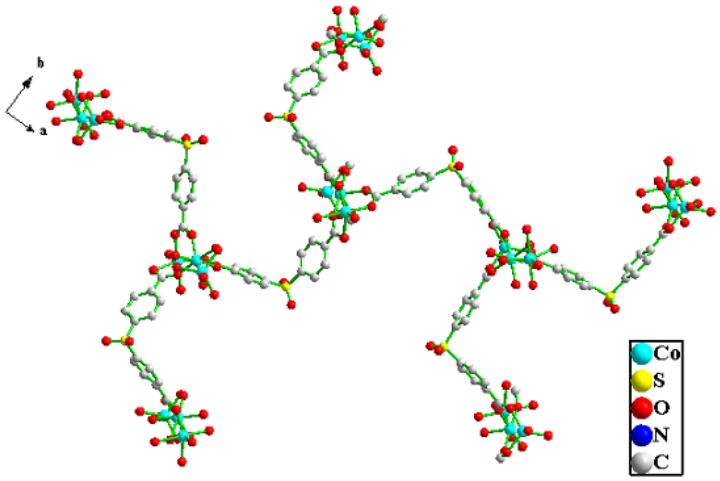


Figure S1. View the 2D zigzag sheet along the c axis in **1**.

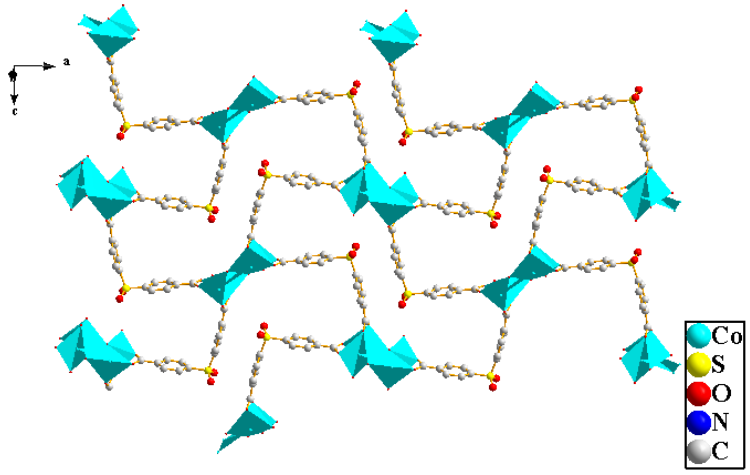
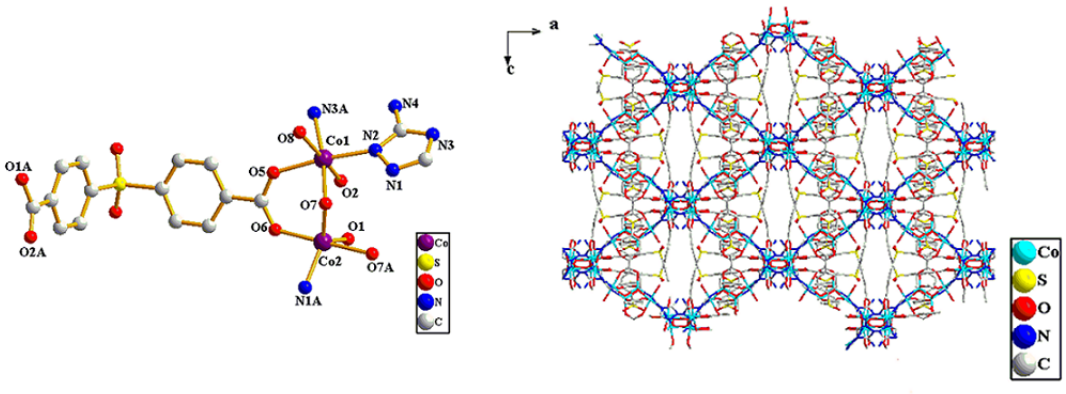


Figure S2. View the 2D sheet in ac plane of **2**.



a b

Figure S3. (a) Coordination environment of Co(II) ion in **3** with hydrogen atoms omitted for clarity. (b) View the 3D "onion" framework along the b axis in **3**.

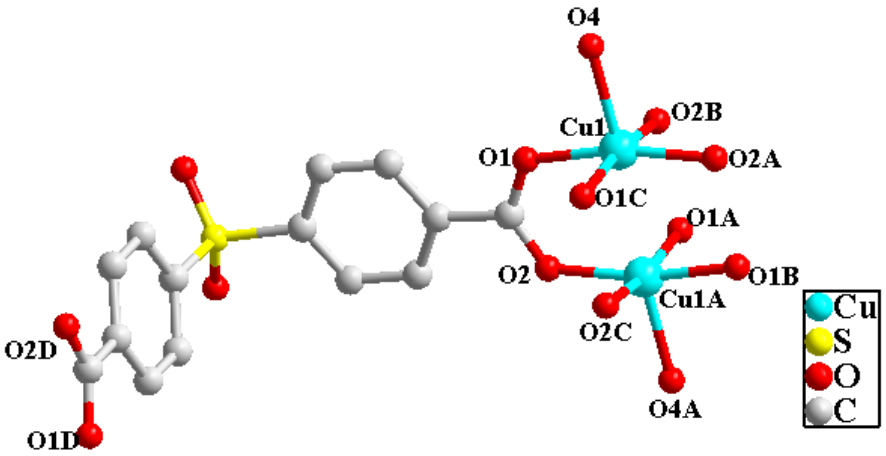


Figure S4. Coordination environment of Cu(II) ion in **5** with hydrogen atoms omitted for clarity.

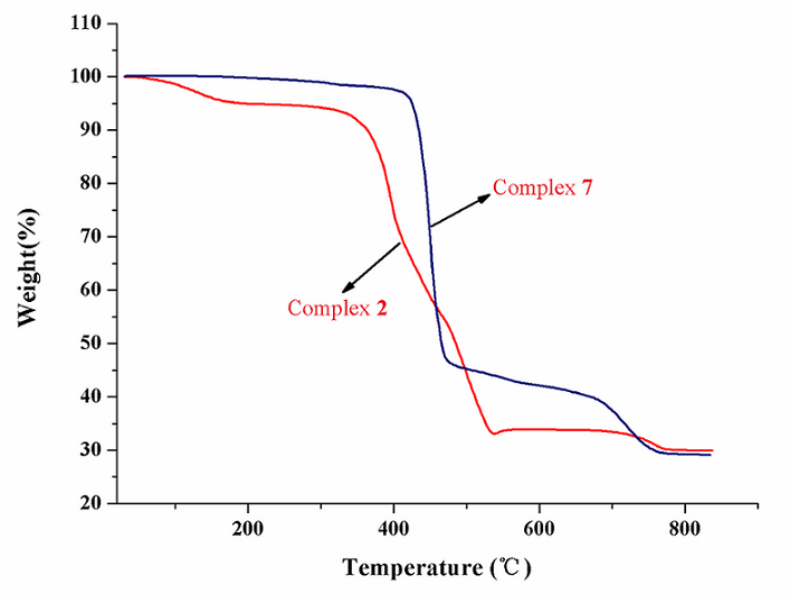


Figure S5. TGA curves of complexes **2** and **7**.

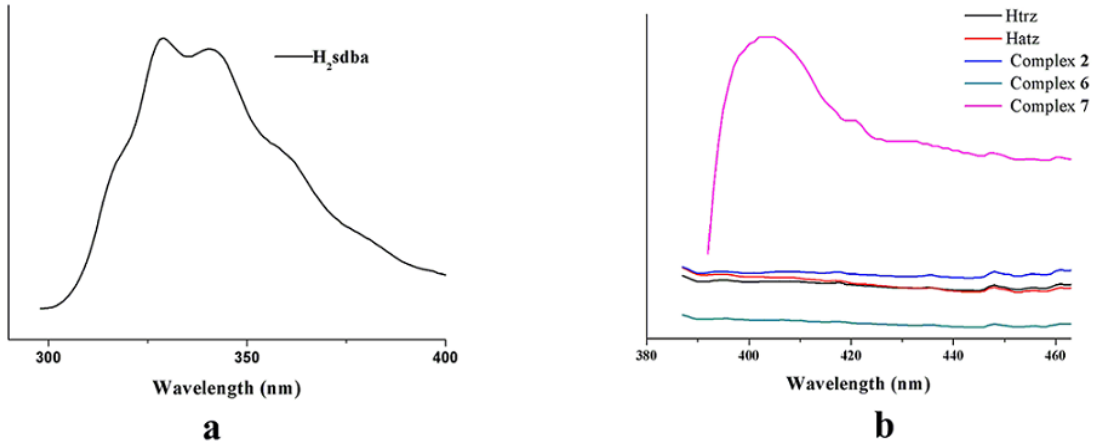


Figure S6. Solid-state photoluminescent spectra of **2**, **6**, **7** and corresponding ligands at room temperature.