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Multi-functional d^{10} metal-organic materials based on bis-pyrazole/pyridine ligands-supported by 2,6-di(3-pyrazolyl)pyridine with different spanning flexible dicarboxylate ligands: Synthesis, structure, photoluminescent and catalytic properties

Xiaoxi Zhang[1], Na Xing[1], Fengying Bai*[2], Lijuan Wan[1], Hui Shan[1], Yanan Hou[1], Yongheng Xing*[1], Zhan Shi[3]

[1] *College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian City, 11602*

[2] *College of Life Science, Liaoning Normal University, Dalian City, 11602*

[3] *State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, P.R. China*

*e-mail: xingyongheng2000@163.com tel: 0411-82156987

Table S1. Selected bond lengths (Å) and angles (°) of the complexes **1-6**

Complex **1**					
Zn1-O3	2.058(4)	Zn1-N4	2.239(5)	Zn2-O4	2.059(4)
Zn1-O1	2.081(4)	Zn1-N2	2.194(5)	Zn2-O4$^{\#}$	2.059(4)
Zn1-O2	2.130(4)	Zn2-O5	2.103(4)	Zn2-O5$^{\#}$	2.103(4)
Zn1-N3	2.096(4)	Zn2-O7	2.159(4)	Zn2-O7$^{\#}$	2.159(4)
O3-Zn1-O1	90.08(17)	O2-Zn1-N2	94.16(17)	O4-Zn2-O5	96.68(16)
O3-Zn1-O2	78.53(15)	O3-Zn1-N4	103.97(18)	O4$^{\#}$-Zn2-O5	95.95(16)
O1-Zn1-O2	168.61(15)	N3-Zn1-N4	74.59(18)	O5$^{\#}$-Zn2-O5	79.3(2)
O3-Zn1-N3	167.49(17)	N3-Zn1-N2	75.36(18)	O4-Zn2-O7	90.56(15)
O1-Zn1-N3	102.34(17)	N2-Zn1-N4	149.29(17)	O4$^{\#}$-Zn2-O7	79.12(15)
N3-Zn1-O2	89.04(15)	O5#1-Zn2-O7	89.40(17)	O4-Zn2-O5$^{\#}$	95.95(16)
O3-Zn1-N2	106.74(18)	O5-Zn2-O7	167.17(17)	O4#-Zn2-O5$^{\#}$	96.68(16)
O1-Zn1-N2	89.13(18)	O4-Zn2-O4#	163.6(2)	O5#-Zn2-O7$^{\#}$	167.16(17)
O1-Zn1-N4	91.17(17)	O4-Zn2-O7#	79.12(15)	O5-Zn2-O7$^{\#}$	89.40(17)
O2-Zn1-N4	91.54(16)	O4#-Zn2-O7#	90.56(15)	O7-Zn2-O7$^{\#}$	102.4(2)
Complex **2**					
Zn-O1	1.936(3)	Zn-N3	2.113(5)	Zn-N2$^{\#1}$	2.234(3)
Zn-O1$^{\#1}$	1.936(3)	Zn-N2	2.234(3)	O1-Zn-O1$^{\#1}$	134.3(2)
O1-Zn-N3	112.85(10)	O1$^{\#1}$-Zn-N2	102.88(12)	O1#1-Zn-N2$^{\#1}$	89.43(12)
O1#1-Zn-N3	112.85(10)	N3-Zn-N2	74.09(9)	N3-Zn-N2$^{\#1}$	74.09(9)
O1-Zn-N2	89.43(12)	O1-Zn-N2$^{\#1}$	102.88(12)	N2-Zn-N2$^{\#1}$	148.17(19)
Complex **3**					
Zn1-O2	2.001(2)	Zn1-N2	2.221(3)	Zn2-N8	2.104(3)
Zn1-N10	2.001(3)	Zn2-O1	1.987(3)	Zn2-N9	2.136(3)
Zn1-N3	2.113(3)	Zn2-N5	2.013(3)	Zn2-N7	2.255(3)
Zn1-N4	2.142(3)	O2-Zn1-N10	107.54(11)	O2-Zn1-N3	124.23(11)
N10-Zn1-N3	128.14(12)	N3-Zn1-N2	74.04(10)	N5-Zn2-N9	97.23(11)
O2-Zn1-N4	96.86(11)	N4-Zn1-N2	148.67(10)	N8-Zn2-N9	75.15(11)
N10-Zn1-N4	97.66(12)	O1-Zn2-N5	106.25(11)	O1-Zn2-N7	94.72(11)
N3-Zn1-N4	75.05(11)	O1-Zn2-N8	119.77(11)	N5-Zn2-N7	107.27(11)
O2-Zn1-N2	96.24(11)	N5-Zn2-N8	133.84(12)	N8-Zn2-N7	73.97(11)
N10-Zn1-N2	105.28(11)	O1-Zn2-N9	96.67(11)	N9-Zn2-N7	148.80(11)
Complex **4**					
Zn1-O2	1.966(2)	Zn1-N9	2.305(3)	Zn2-N3	2.114(3)

Zn1-N1	2.005(3)	Zn2-O4	1.970(2)	Zn2-N2	2.191(3)
Zn1-N8	2.123(3)	Zn2-N6	2.003(3)	Zn2-N4	2.238(3)
Zn1-N7	2.172(3)	O2-Zn1-N1	118.99(10)	O2-Zn1-N8	111.43(10)
N1-Zn1-N8	129.26(10)	N8-Zn1-N9	73.09(10)	N6-Zn2-N2	90.56(10)
O2-Zn1-N7	99.18(10)	N7-Zn1-N9	147.60(10)	N3-Zn2-N2	75.14(10)
N1-Zn1-N7	91.69(10)	O4-Zn2-N6	116.93(11)	O4-Zn2-N4	94.40(10)
N8-Zn1-N7	74.66(10)	O4-Zn2-N3	116.72(10)	N6-Zn2-N4	107.13(11)
O2-Zn1-N9	95.33(10)	N6-Zn2-N3	126.10(11)	N3-Zn2-N4	73.45(10)
N1-Zn1-N9	106.30(10)	O4-Zn2-N2	100.49(10)	N2-Zn2-N4	148.58(10)
Complex **5**					
Zn1-O1	1.994(6)	Zn1-N9	2.234(7)	Zn2-N3	2.120(7)
Zn1-N1	2.005(7)	Zn2-N6	1.997(8)	Zn2-N2	2.125(7)
Zn1-N8	2.099(7)	Zn2-O2	2.009(6)	Zn2-N4	2.157(7)
Zn1-N7	2.149(7)	O1-Zn1-N1	107.6(3)	O1-Zn1-N8	122.6(3)
N1-Zn1-N8	129.8(3)	N8-Zn1-N9	74.6(3)	O2-Zn2-N2	96.6(3)
O1-Zn1-N7	99.7(3)	N7-Zn1-N9	149.8(3)	N3-Zn2-N2	74.6(3)
N1-Zn1-N7	96.1(3)	N6-Zn2-O2	105.9(3)	N6-Zn2-N4	106.0(3)
N8-Zn1-N7	75.3(3)	N6-Zn2-N3	132.5(3)	O2-Zn2-N4	95.4(3)
O1-Zn1-N9	94.2(3)	O2-Zn2-N3	121.5(3)	N3-Zn2-N4	74.7(3)
N1-Zn1-N9	105.1(3)	N6-Zn2-N2	98.0(3)	N2-Zn2-N4	149.0(3)
Complex **6**					
Zn1-N10	1.989(2)	Zn1-N4	2.189(3)	Zn2-N8	2.082(2)
Zn1-O1	2.000(2)	Zn2-O2	2.008(2)	Zn2-N9	2.158(3)
Zn1-N3	2.096(2)	Zn2-N5	2.017(2)	Zn2-N7	2.171(3)
Zn1-N2	2.187(3)	N10-Zn1-O1	109.02(10)	N10-Zn1-N3	131.39(11)
O1-Zn1-N3	118.91(9)	N3-Zn1-N4	75.25(10)	N5-Zn2-N9	92.98(10)
N10-Zn1-N2	111.25(10)	N2-Zn1-N4	148.99(9)	N8-Zn2-N9	75.98(10)
O1-Zn1-N2	93.46(10)	O2-Zn2-N5	109.65(10)	O2-Zn2-N7	100.88(10)
N3-Zn1-N2	74.79(10)	O2-Zn2-N8	120.91(10)	N5-Zn2-N7	105.13(10)
N10-Zn1-N4	94.55(10)	N5-Zn2-N8	128.54(11)	N8-Zn2-N7	75.46(10)
O1-Zn1-N4	94.04(10)	O2-Zn2-N9	93.37(10)	N9-Zn2-N7	151.40(9)

Table S2. Bond distances (Å) and angles (°) of hydrogen bonds in the complexes **1-6**

D—H---A	*d(D-H)*	*D(H---A)*	*dD((D---A)*	*∠DHA*
Complex **1**				
N1—H1D---O7	0.8600	2.0375	2.8457	156.22
O1—H1E---O5	0.8501	2.2012	2.9262	143.16
O1—H1F---O1W	0.8500	2.0341	2.6709	131.11
O2W—H2WA---O5	0.9599	1.8789	2.7896	157.43
O2W—H2WB---O1W	0.9601	1.8902	2.6584	135.14
N5—H5A---O6	0.8600	2.0310	2.8794	168.77
C7—H7--- O2W	0.9300	2.3837	3.2712	159.55
C8—H8---O2	0.9300	2.4098	3.2791	155.56
Complex **2**				
N1—H1D---O1W	0.8600	1.9600	2.7918	162.37
O1W—H1WB---O2	0.8499	1.9638	2.7384	151.01
Complex **3**				
N1—H1A---O3	0.8600	1.7973	2.6056	155.79
N6—H6A---O1W	0.8600	1.9285	2.7802	170.40
Complex **4**				
O2W— H2WA---O1	0.8499	1.9482	2.6211	135.27
N5— H5A ---O1W	0.8600	2.2690	3.1227	171.80
N10— H10A---O2W	0.8600	2.0088	2.8384	161.76
C12—H12A---O1	0.9300	2.5267	3.3290	144.65
C39—H39A---O2	0.9300	2.5523	3.3286	141.21
Complex **5**				
N5—H5A---O1W	0.8600	1.9919	2.8191	161.02
N10—H10A---O2W	0.8600	1.9445	2.7812	163.95
Complex **6**				
O1—H1C---O5	0.8457	1.7803	2.6208	172.30
O1—H1D---O2	0.8550	1.8286	2.6772	171.50
O2W—H2WA---O2	0.9267	1.8495	2.7610	167.30
O3W—H3WA---O5	0.8480	1.8381	2.6466	158.83
O1W—H1WB---O2W	0.8596	1.8920	2.6055	139.42
O2W—H2WB---O3W	0.8559	2.0121	2.8157	156.02
O3W—H3WB---O1W	0.8398	2.0822	2.8297	148.02
N1—H1B---O4	0.8600	1.8768	2.7146	164.28

N6—H6A---O3W	0.8600	1.9154	2.7499	163.17
C5—H5A---O4	0.9300	2.4161	3.3118	161.66
C34—H34A---O3	0.9300	2.4042	3.3118	165.14

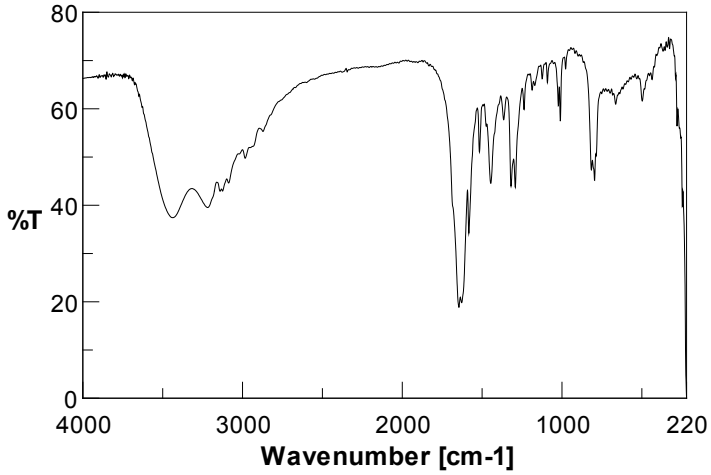

Fig S1. The Solid-state IR spectra of complex **1** at a room temperature

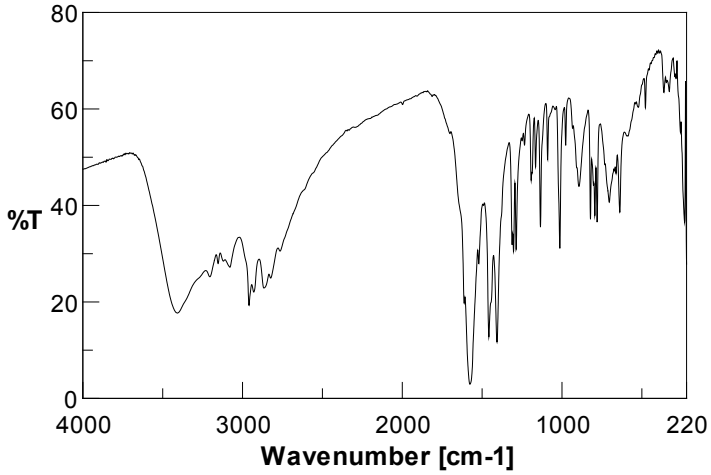

Fig S2. The Solid-state IR spectra of complex **2** at a room temperature

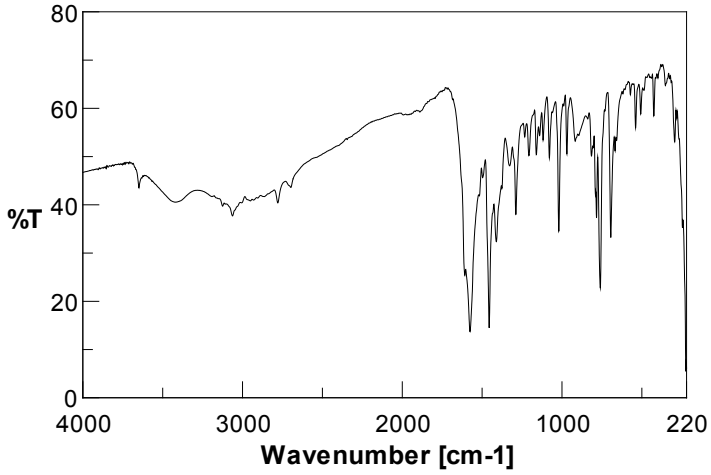

Fig S3. The Solid-state IR spectra of complex 3 at a room temperature

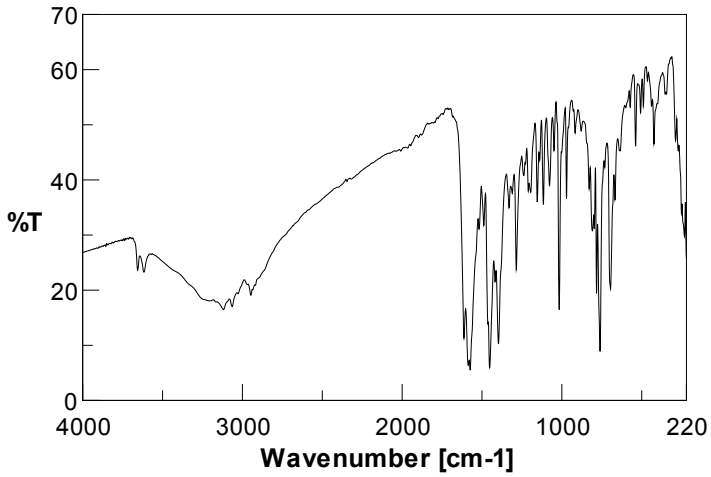

Fig S4. The Solid-state IR spectra of complex **4** at a room temperature

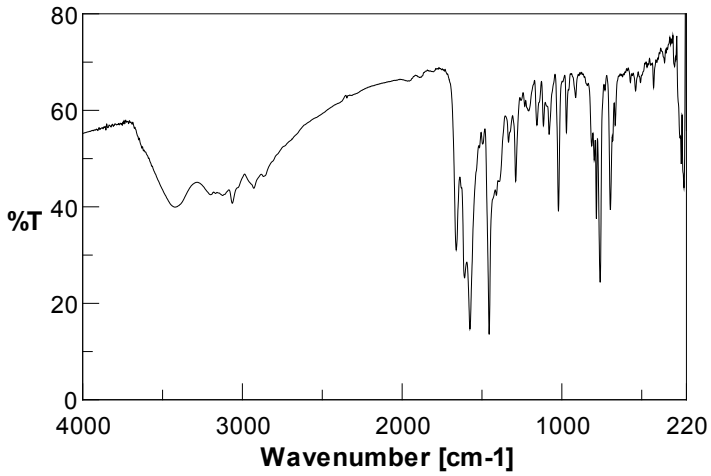

Fig S5. The Solid-state IR spectra of complex **5** at a room temperature

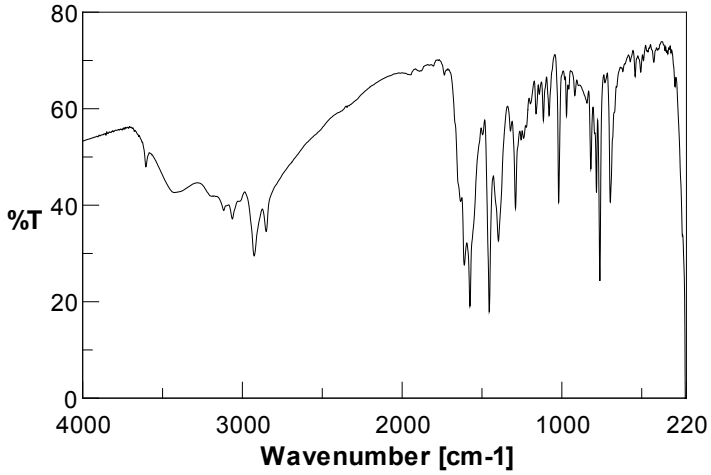

Fig S6. The Solid-state IR spectra of complex **6** at a room temperature

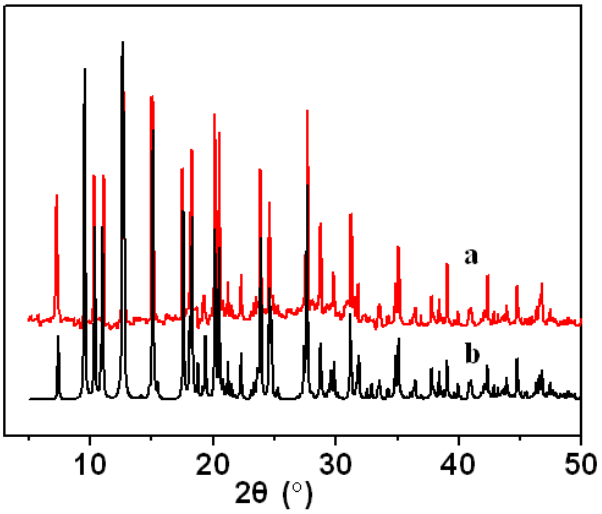

Fig S7. PXRD powder patterns: a experimental PXRD for complex **1**, b the simulated PXRD pattern calculated from single-crystal structure of complex **1**.

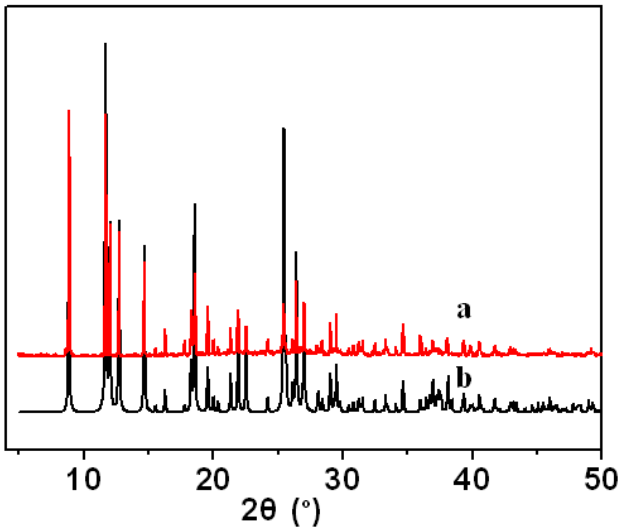

Fig S8. PXRD powder patterns: a experimental PXRD for complex 2, b the simulated PXRD pattern calculated from single-crystal structure of complex 2.

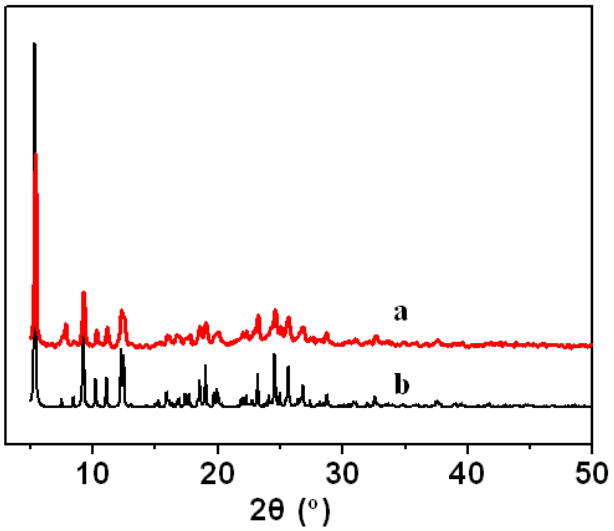

Fig S9. PXRD powder patterns: a experimental PXRD for complex 3, b the simulated PXRD pattern calculated from single-crystal structure of complex 3.

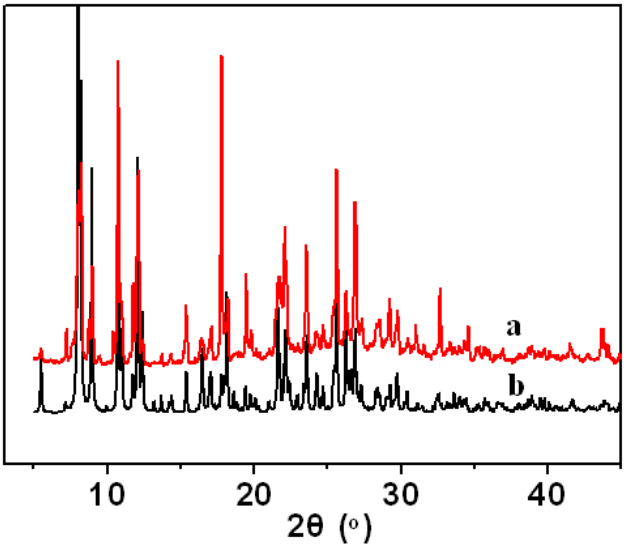

Fig S10. PXRD powder patterns: a experimental PXRD for complex 4, b the simulated PXRD pattern calculated from single-crystal structure of complex 4.

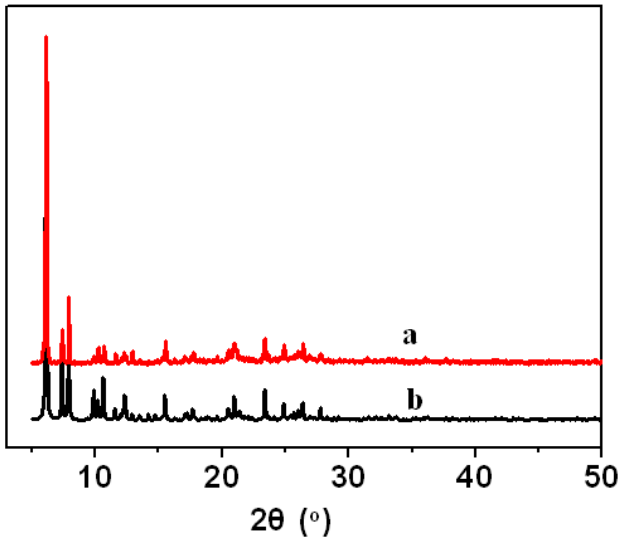

Fig S11. PXRD powder patterns: a experimental PXRD for complex 5, b the simulated PXRD pattern calculated from single-crystal structure of complex 5.

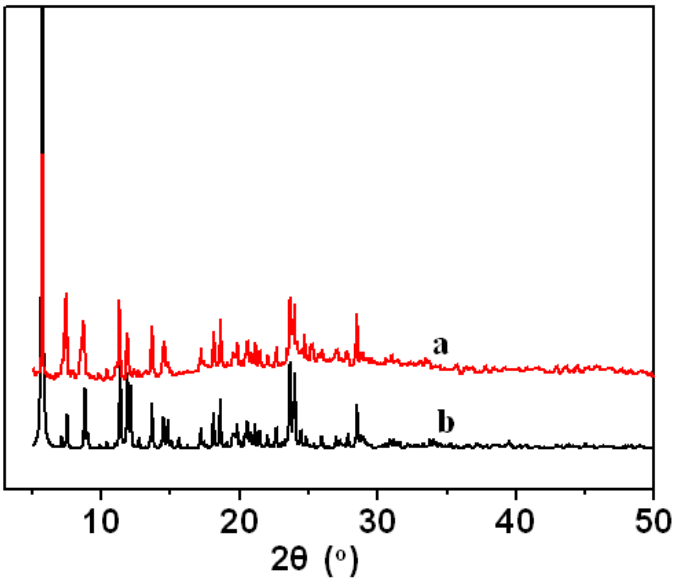

Fig S12. PXRD powder patterns: a experimental PXRD for complex 6, b the simulated PXRD pattern calculated from single-crystal structure of complex 6.

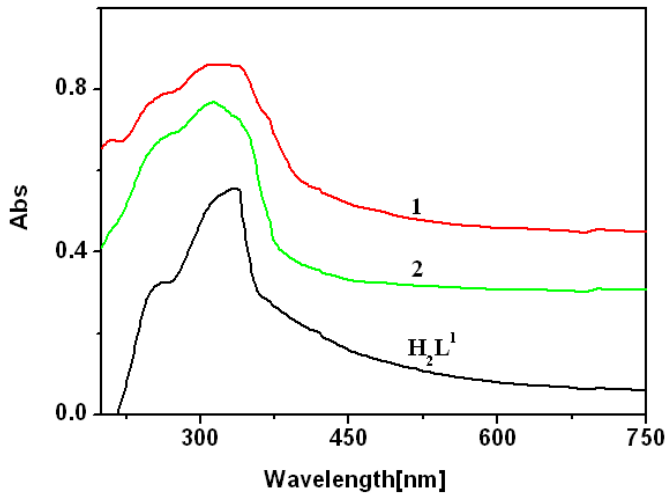

Fig S13. The Solid-state UV–Vis spectra of $H_2L^1$and complex 1, 2 at a room temperature

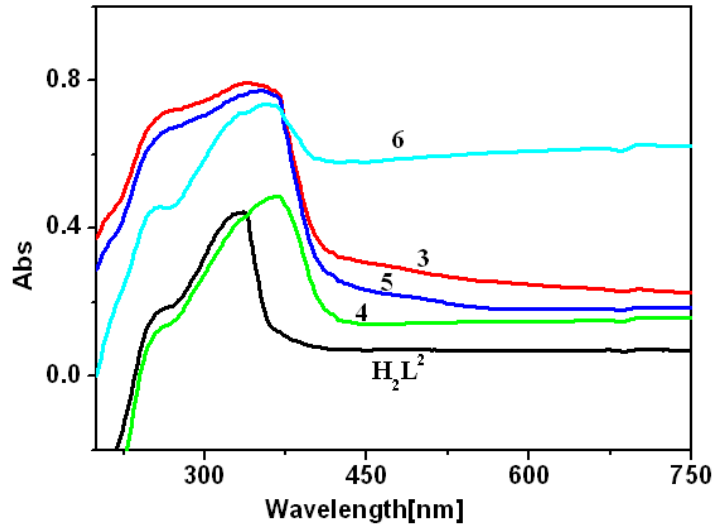

Fig S14. The Solid-state UV–Vis spectra of $H_2L^2$and complex 3-6 at a room temperature

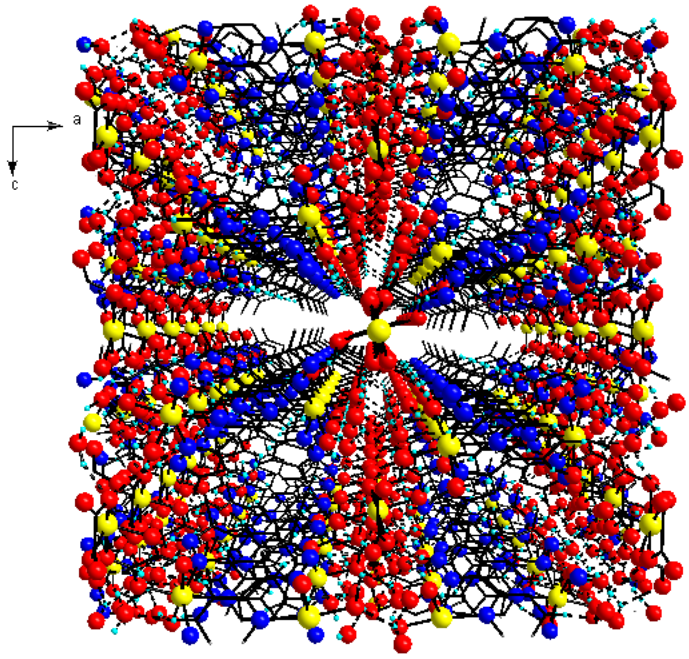

Fig S15. A view of the hydrogen bonds of complex **1** (a part of hydrogen atoms are omitted for clarity)

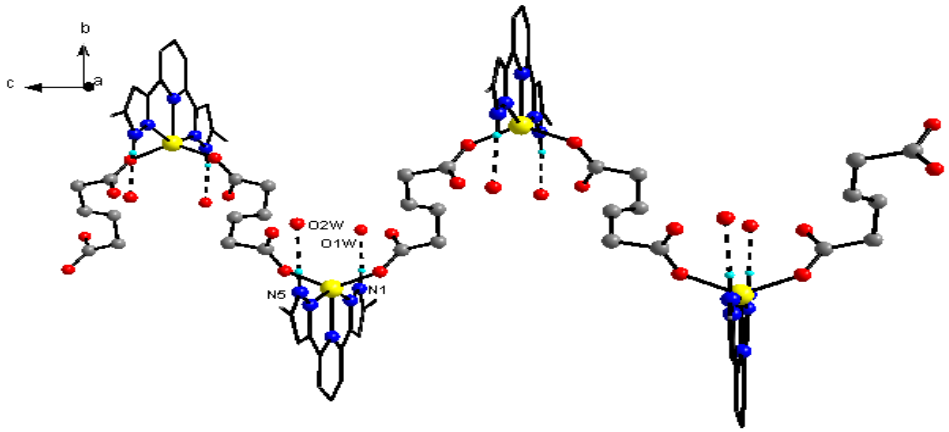

Fig S16. A view of the hydrogen bonds of complex **2** (a part of hydrogen atoms are omitted for clarity)

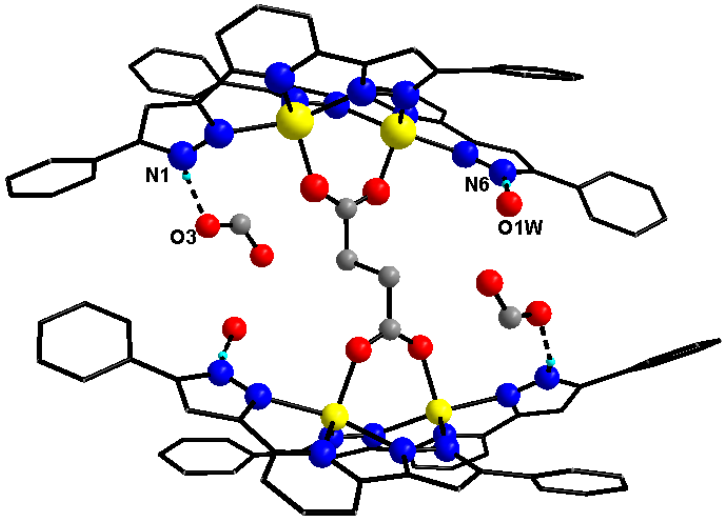

Fig S17. A view of the hydrogen bonds of complex **3** (a part of hydrogen atoms are omitted for clarity)

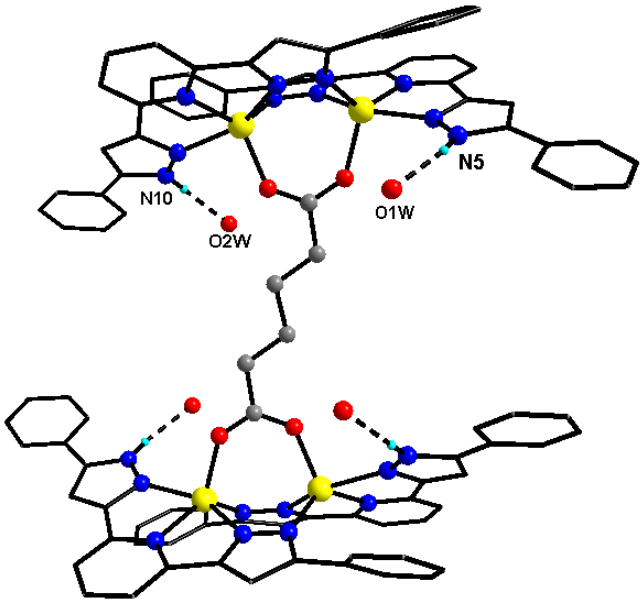

Fig S18. A view of the hydrogen bonds of complex **5** (a part of hydrogen atoms are omitted for clarity