Synthesis of two mononuclear Schiff-base metal (M = Fe, Cu) complexes: MOF structure, dye degradation, H_2O_2 sensing and DNA binding property

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Electronic Supplementary Information

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ESI 1. ^{1}H NMR of the Schiff base ligand

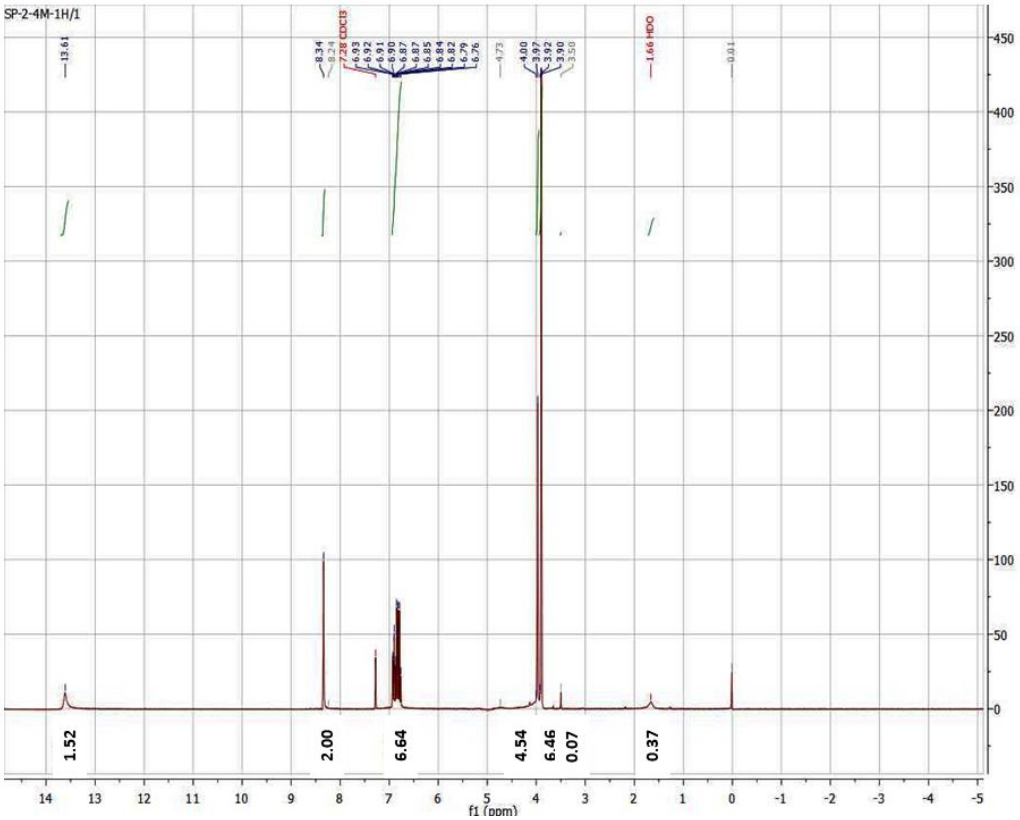

Figure S1: ^{1}HNMR of Schiff base ligand

ESI 2: FT-IR analysis

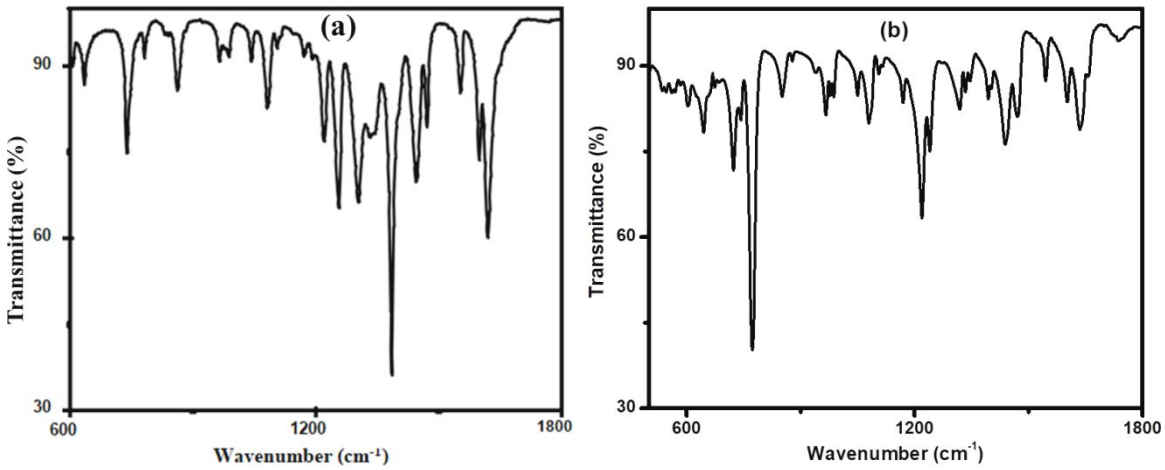

Figure S2. FT-IR of (a) Complex 1 and (b) complex 2

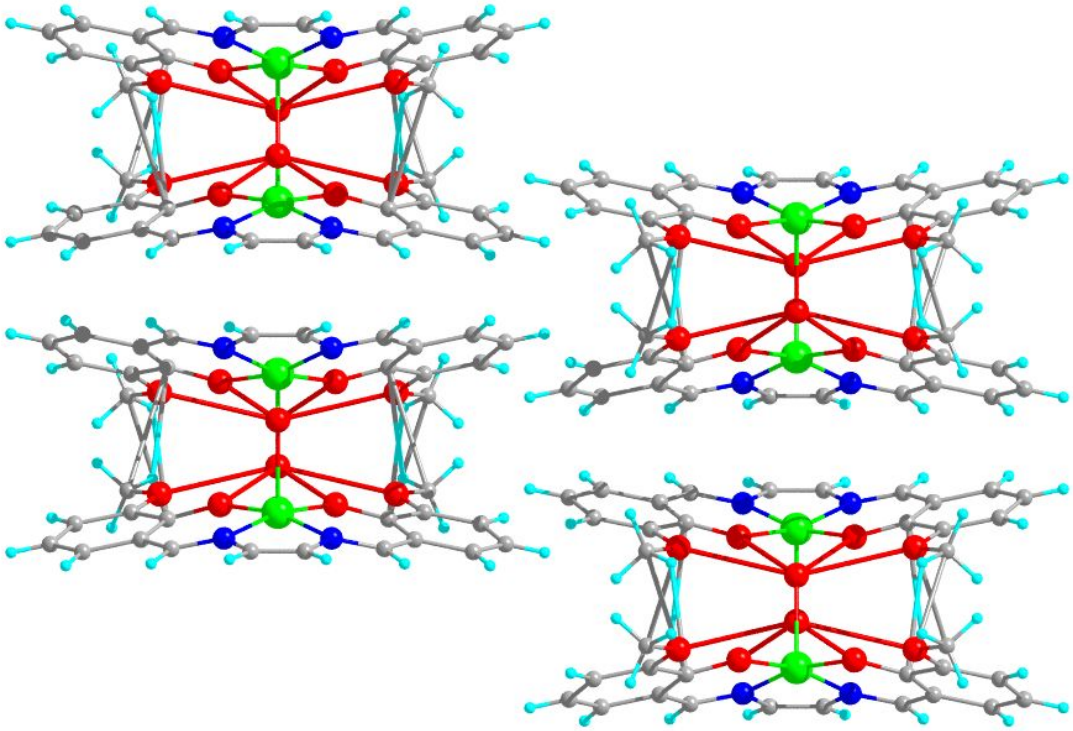

Figure S3: MOF at (100) ‘a’ axis in central projection of complex 2

Table S1. Selected geometric information of the complex 1

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
Fe1—O1	1.882 (16)	C8—C13	1.408(4)
Fe1—O2	1.866 (21)	C8—C9	1.415(4)
Fe1—O5	2.316 (13)	C13—C14	1.438(5)
Fe1—O6	2.088 (26)	C13—C12	1.413(4)
Fe1—N1	2.094 (26)	C7—H7	0.9300
Fe1—N2	2.075 (27)	C9—C10	1.382(5)
O1—C1	1.316(3)	C3—H3	0.9300
O5—H5A	0.8504	C3—C4	1.384(5)
O5—H5B	0.8503	C5—H5	0.9300
O2—C8	1.320(3)	C5—C4	1.370(5)
O3—C2	1.361(3)	C14—H14	0.9300
O3—C17	1.420(3)	C4—H4	0.9300
O4—C9	1.356(4)	C17—H17A	0.9600
O4—C18	1.423(4)	C17—H17B	0.9600
O6—H6A	0.8507	C17—H17C	0.9600
O6—H6B	0.8505	C12—H12	0.9300
N1—C7	1.285(4)	C12—C11	1.377(7)
N1—C15	1.473(4)	C10—H10	0.9300
N2—C14	1.284(4)	C10—C11	1.391(6)
N2—C16	1.478(4)	C11—H11	0.9300
N3—O8	1.226(4)	C16—H16A	0.9700
N3—O9	1.196(4)	C16—H16B	0.9700
N3—O7	1.204(4)	C16—C15	1.485(6)
C1—C2	1.410(3)	C15—H15A	0.9700
C1—C6	1.407(4)	C15—H15B	0.9700
C2—C3	1.379(4)	C18—H18A	0.9600
C6—C7	1.437(4)	C18—H18B	0.9600
C6—C5	1.414(4)	C18—H18C	0.9600

Atoms 1,2,3	Angle 1,2,3 [°]	Atoms 1,2,3	Angle 1,2,3 [°]
O1—Fe1—O5	89.57(8)	N1—C7—H7	117.400
O1—Fe1—O2	101.45(8)	C6—C7—H7	117.400
O1—Fe1—O6	93.26(9)	O4—C9—C8	113.7(3)
O1—Fe1—N1	88.99(8)	O4—C9—C10	126.4(3)
O1—Fe1—N2	168.06(9)	C10—C9—C8	119.9(3)
O2—Fe1—O5	92.04(8)	C2—C3—H3	119.900
O2—Fe1—O6	91.91(9)	C2—C3—C4	120.3(3)
O2—Fe1—N1	169.56(9)	C4—C3—H3	119.900
O2—Fe1—N2	89.63(9)	C6—C5—H5	119.800
O6—Fe1—O5	174.60(9)	C4—C5—C6	120.5(3)
O6—Fe1—N1	87.28(10)	C4—C5—H5	119.800
N1—Fe1—O5	88.17(8)	N2—C14—C13	125.5(3)
N2—Fe1—O5	85.57(9)	N2—C14—H14	117.200
N2—Fe1—O6	90.77(10)	C13—C14—H14	117.200
N2—Fe1—N1	79.98(9)	C3—C4—H4	119.600
C1—O1—Fe1	132.62(15)	C5—C4—C3	120.8(3)

Fe1—O5—H5A	109.300	C5—C4—H4	119.600
Fe1—O5—H5B	109.500	O3—C17—H17A	109.500
H5A—O5—H5B	109.500	O3—C17—H17B	109.500
C8—O2—Fe1	131.50(18)	O3—C17—H17C	109.500
C2—O3—C17	118.0(2)	H17A—C17—H17B	109.500
C9—O4—C18	118.3(3)	H17A—C17—H17C	109.500
Fe1—O6—H6A	109.400	H17B—C17—H17C	109.500
Fe1—O6—H6B	109.400	C13—C12—H12	119.800
H6A—O6—H6B	109.400	C11—C12—C13	120.3(4)
C7—N1—Fe1	125.76(18)	C11—C12—H12	119.800
C7—N1—C15	121.1(2)	C9—C10—H10	119.900
C15—N1—Fe1	112.8(2)	C9—C10—C11	120.2(4)
C14—N2—Fe1	125.1(2)	C11—C10—H10	119.900
C14—N2—C16	121.9(3)	C12—C11—C10	121.0(3)
C16—N2—Fe1	112.9(2)	C12—C11—H11	119.500
O9—N3—O8	123.6(4)	C10—C11—H11	119.500
O9—N3—O7	116.7(4)	N2—C16—H16A	109.700
O7—N3—O8	119.7(4)	N2—C16—H16B	109.700
O1—C1—C2	116.9(2)	N2—C16—C15	109.8(3)
O1—C1—C6	123.8(2)	H16A—C16—H16B	108.200
C6—C1—C2	119.3(2)	C15—C16—H16A	109.700
O3—C2—C1	114.0(2)	C15—C16—H16B	109.700
O3—C2—C3	125.7(2)	N1—C15—C16	110.0(3)
C3—C2—C1	120.3(3)	N1—C15—H15A	109.700
C1—C6—C7	123.5(2)	N1—C15—H15B	109.700
C1—C6—C5	118.8(3)	C16—C15—H15A	109.700
C5—C6—C7	117.6(3)	C16—C15—H15B	109.700
O2—C8—C13	123.5(3)	H15A—C15—H15B	108.200
O2—C8—C9	116.6(3)	O4—C18—H18A	109.500
C13—C8—C9	119.9(3)	O4—C18—H18B	109.500
C8—C13—C14	123.5(3)	O4—C18—H18C	109.500
C8—C13—C12	118.7(3)	H18A—C18—H18B	109.500
C12—C13—C14	117.7(3)	H18A—C18—H18C	109.500
N1—C7—C6	125.3(2)	H18B—C18—H18C	109.500

Table S2. Selected geometric information of the complex 2

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
Cu1-N1/N1'	1.942(45),	C007—C009	1.434(6)
Cu1-O1/O1'	1.932(28)	C008—C00B	1.379(7)
Cu1-O3	2.330(28)	C009—C00C	1.420(7)
Cu1-N1/N1'	1.942(45),	C00A—H00A	0.9800
Cu1-O1/O1'	1.932(28)	C00A—H00B	0.9800
O1—C006	1.309(5)	C00A—H00C	0.9800
O2—C008	1.369(5)	C00B—H00D	0.9500
O2—C00A	1.423(5)	C00B—C00D	1.384(8)
N1—C007	1.285(7)	C00C—H00E	0.9500
N1—C00E	1.450(6)	C00C—C00D	1.356(8)
C006—C008	1.427(6)	C00D—H00F	0.9500
C006—C009	1.411(6)	C00E—C00E^{i}	1.289(14)
C007—H007	0.9500	C00E—H00G	0.9500

Atoms 1,2,3	Angle 1,2,3 [°]	Atoms 1,2,3	Angle 1,2,3 [°]
O1—Cu1—O1^{i}	90.48(16)	C00B—C008—C006	121.5(4)
O1^{i}—Cu1—O3	98.47(11)	C006—C009—C007	122.4(4)
O1—Cu1—O3	98.42(11)	C006—C009—C00C	120.8(4)
O1—Cu1—N1	92.30(15)	C00C—C009—C007	116.8(4)
O1—Cu1—N1^{i}	166.99(18)	O2—C00A—H00A	109.500
O1^{i}—Cu1—N1^{i}	92.30(15)	O2—C00A—H00B	109.500
O1^{i}—Cu1—N1	167.01(18)	O2—C00A—H00C	109.500
N1—Cu1—O3	93.67(17)	H00A—C00A—H00B	109.500
N1^{i}—Cu1—O3	93.73(17)	H00A—C00A—H00C	109.500
N1^{i}—Cu1—N1	82.3(3)	H00B—C00A—H00C	109.500
C006—O1—Cu1	126.6(3)	C008—C00B—H00D	119.400
C008—O2—C00A	116.8(3)	C008—C00B—C00D	121.3(5)
C007—N1—Cu1	127.5(3)	C00D—C00B—H00D	119.400
C007—N1—C00E	120.0(4)	C009—C00C—H00E	119.500
C00E—N1—Cu1	112.2(4)	C00D—C00C—C009	121.0(4)
O1—C006—C008	118.1(4)	C00D—C00C—H00E	119.500
O1—C006—C009	125.9(4)	C00B—C00D—H00F	120.300
C009—C006—C008	116.0(4)	C00C—C00D—C00B	119.3(5)
N1—C007—H007	117.500	C00C—C00D—H00F	120.300
N1—C007—C009	125.0(4)	N1—C00E—H00G	122.100
C009—C007—H007	117.500	C00E^{i}—C00E—N1	115.8(3)
O2—C008—C006	113.4(4)	C00E^{i}—C00E—H00G	122.100
O2—C008—C00B	125.1(4)		