Supporting Information

Hydrothermal Synthesis and Structural Characterization of Metal−Organic Frameworks Based on Novel Tetradentate Ligands

Yue Liang, Wei-Guan Yuan, Shu-Fang Zhang, Zhan He, Junru Xue, Xia Zhang, Lin-Hai Jing, Da-Bin Qin*

Key Laboratory of Chemical Synthesis and Pollution Control of Sichuan Province, School of Chemistry and Chemical Engineering, China West Normal University, Nanchong 637002, P. R. China.

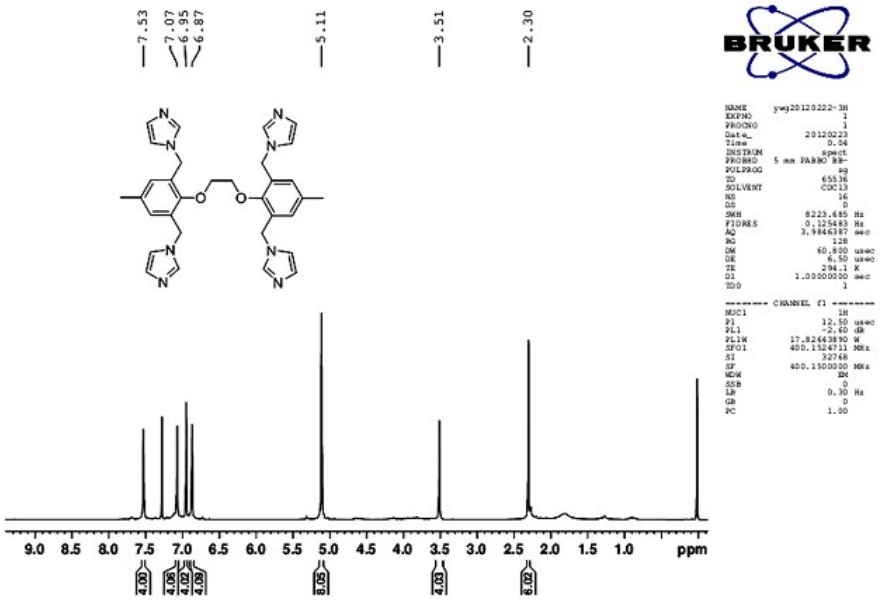

Figure S1. ^{1}H NMR spectra of ligand **L1**

* corresponding author. E-mail: qdbkyl@cwnu.edu.cn; Fax: (+86)-817-256-8081.

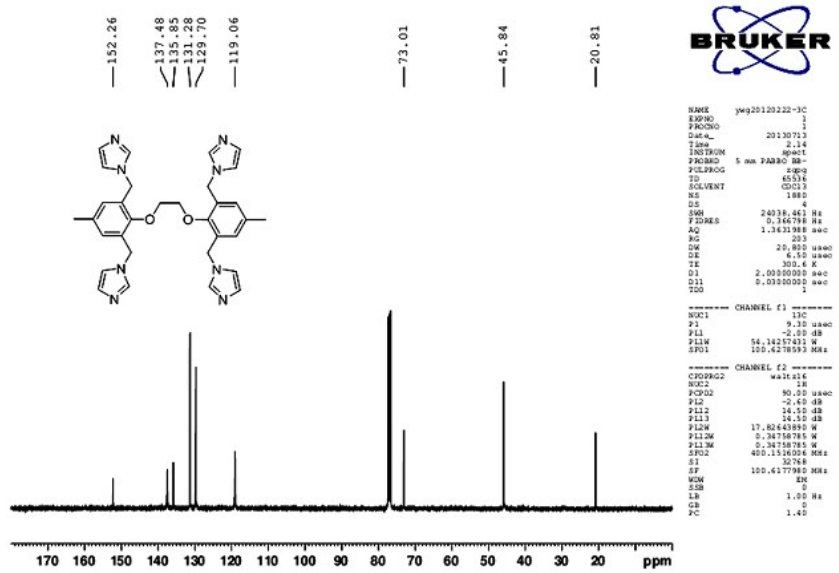

Figure S2. ^{13}C NMR spectra of ligand **L1**

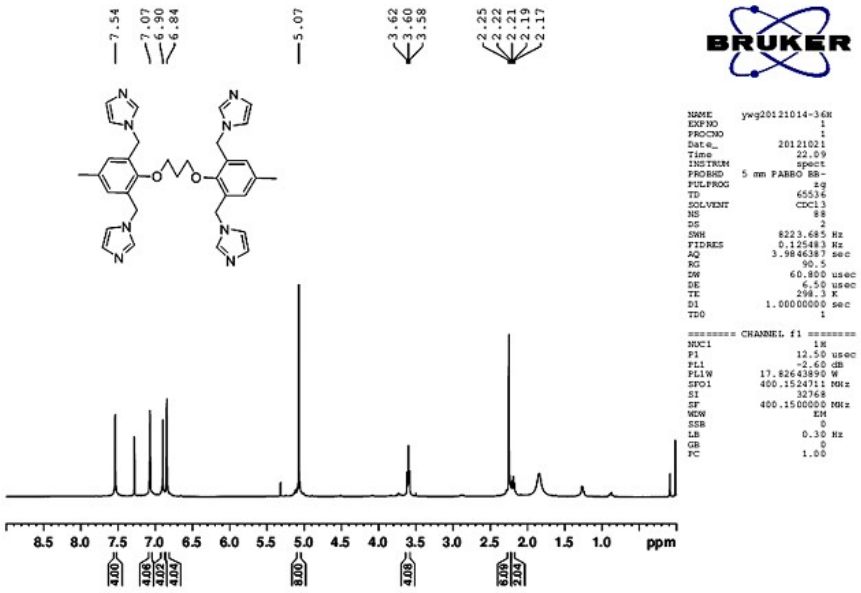

Figure S3. ^{1}H NMR spectra of ligand **L2**

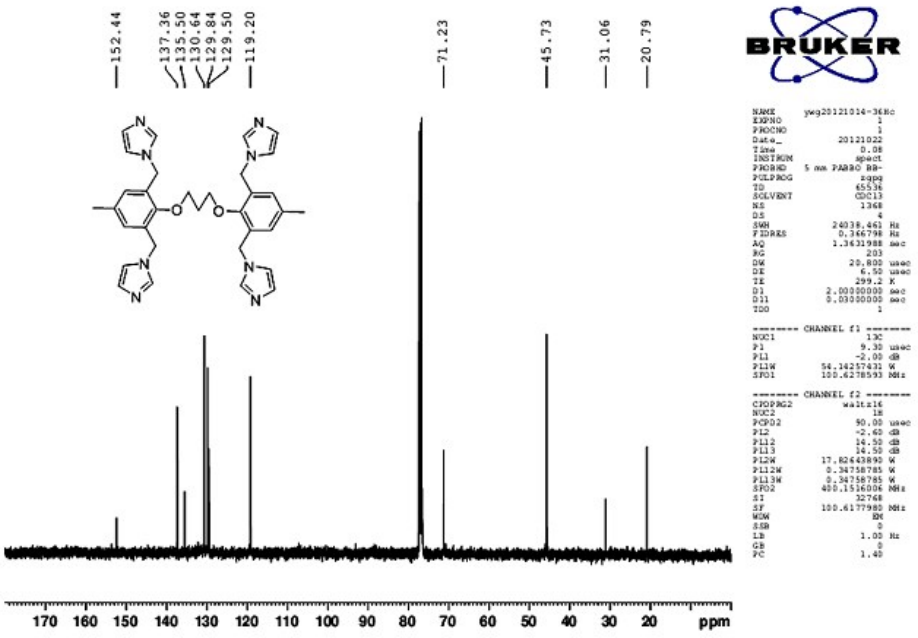

Figure S4. ^{13}C NMR spectra of ligand **L2**

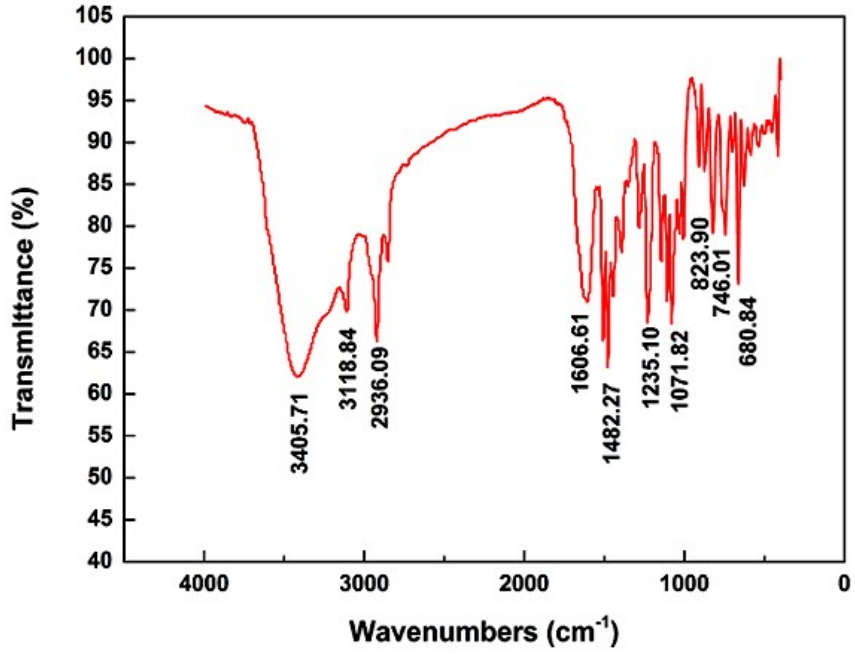

Figure S5. IR spectra of L1

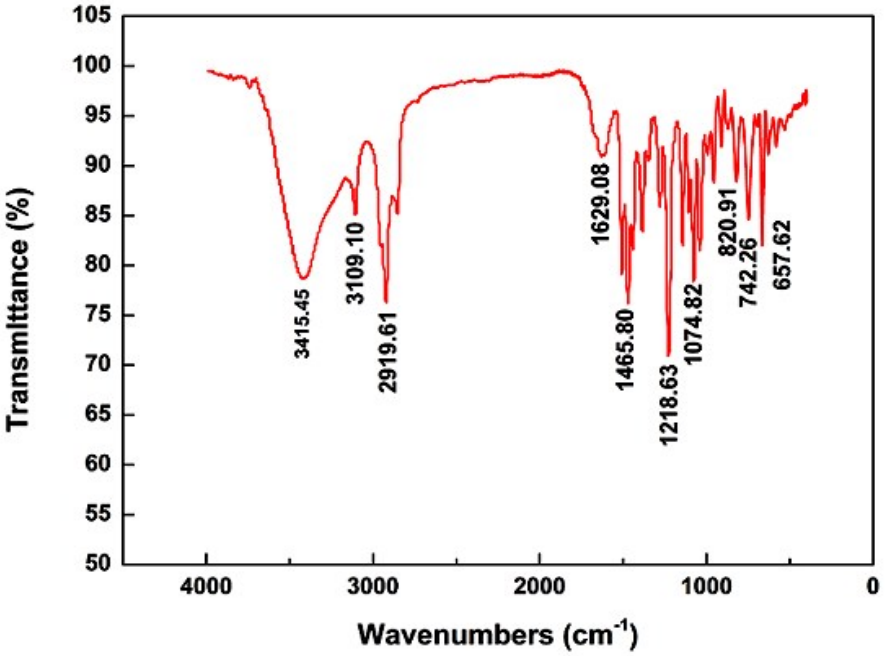

Figure S6. IR spectra of L2

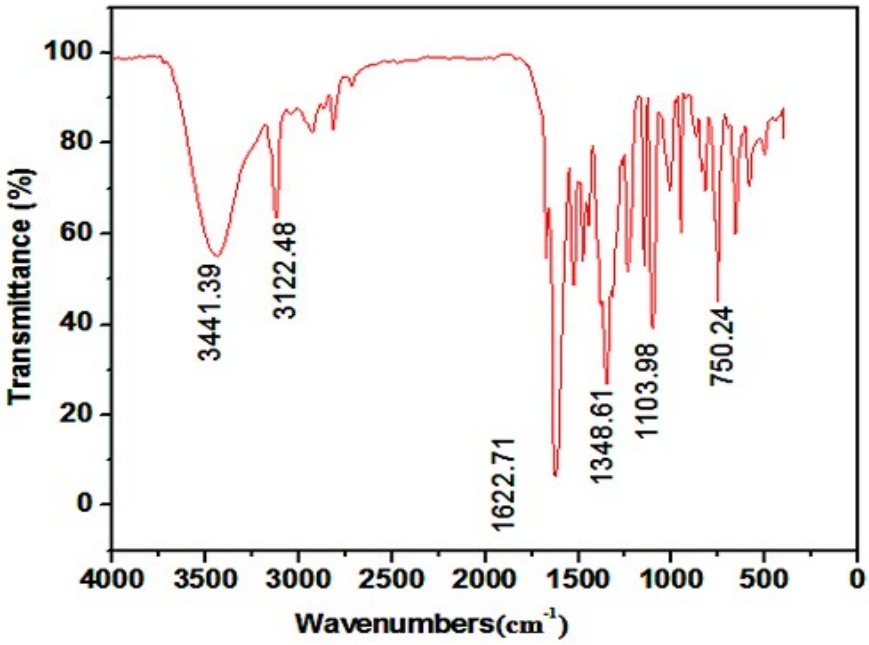

Figure S7. IR spectra of complex **1**

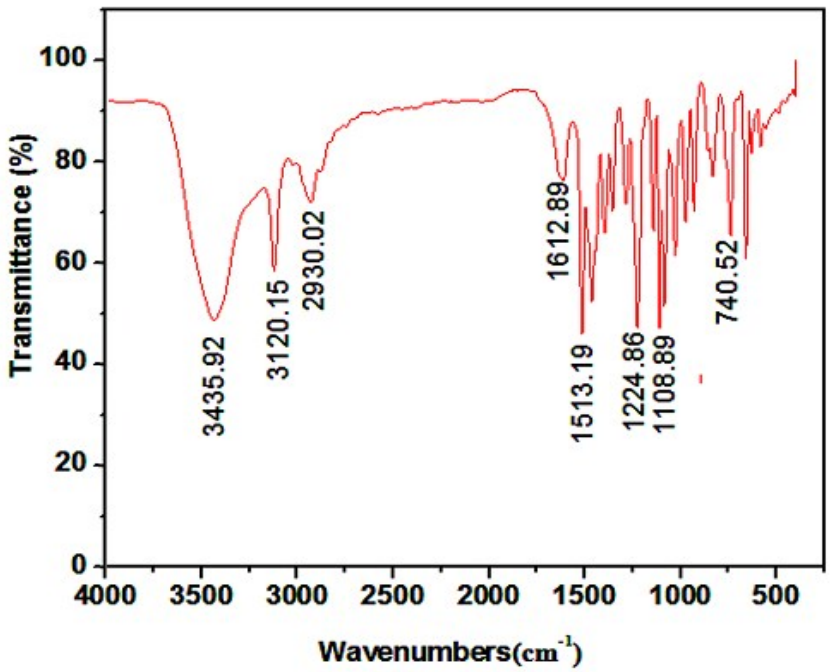

Figure S8. IR spectra of complex **2**

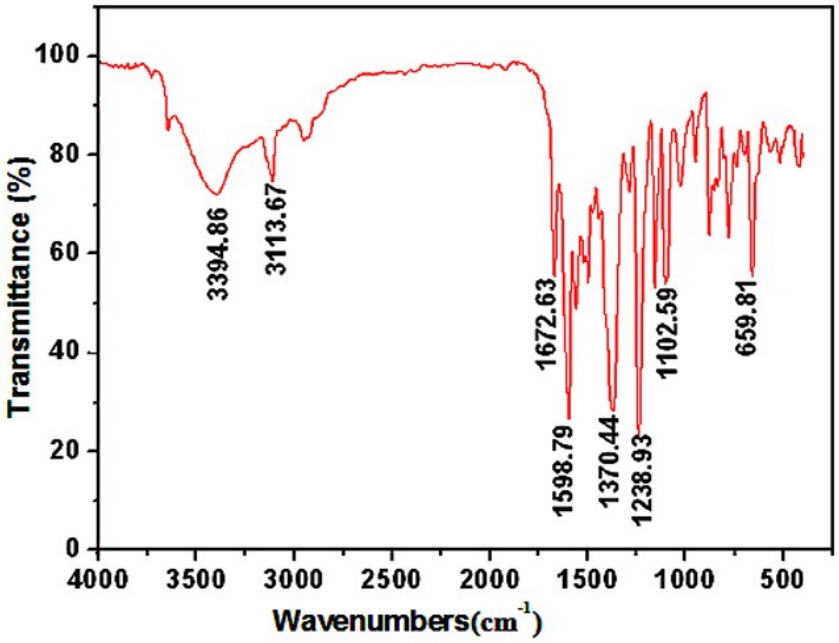

Figure S9. IR spectra of complex **3**

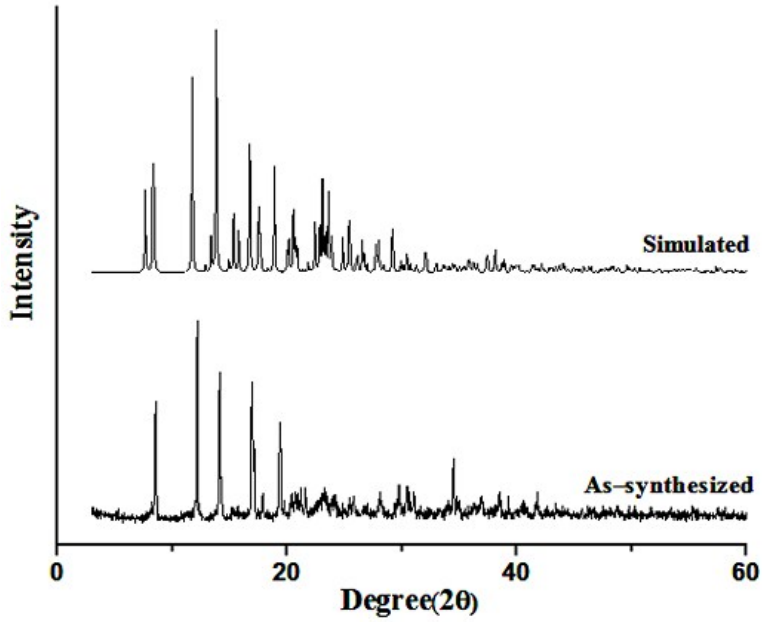

Figure S10. Powder X-ray diffraction patterns of complex **1**

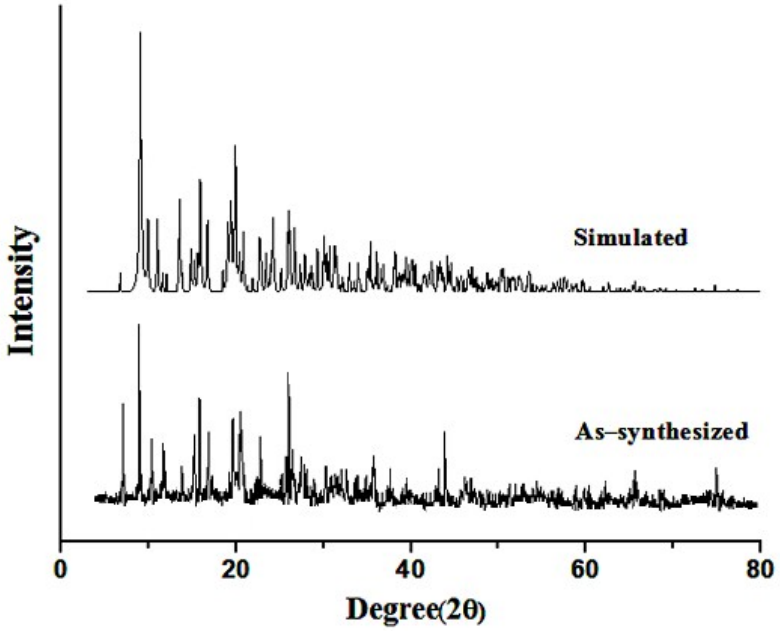

Figure S11. Powder X-ray diffraction patterns of complex **2**

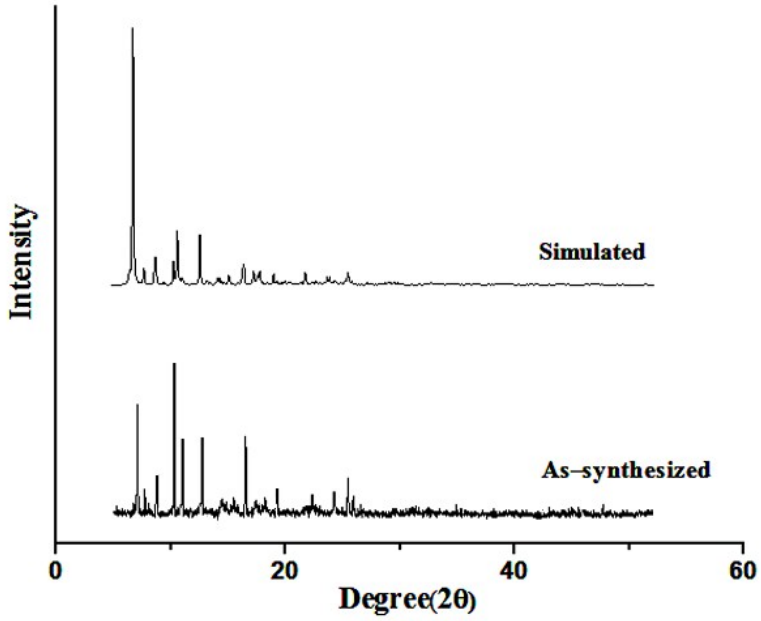

Figure S12. Powder X-ray diffraction patterns of complex **3**

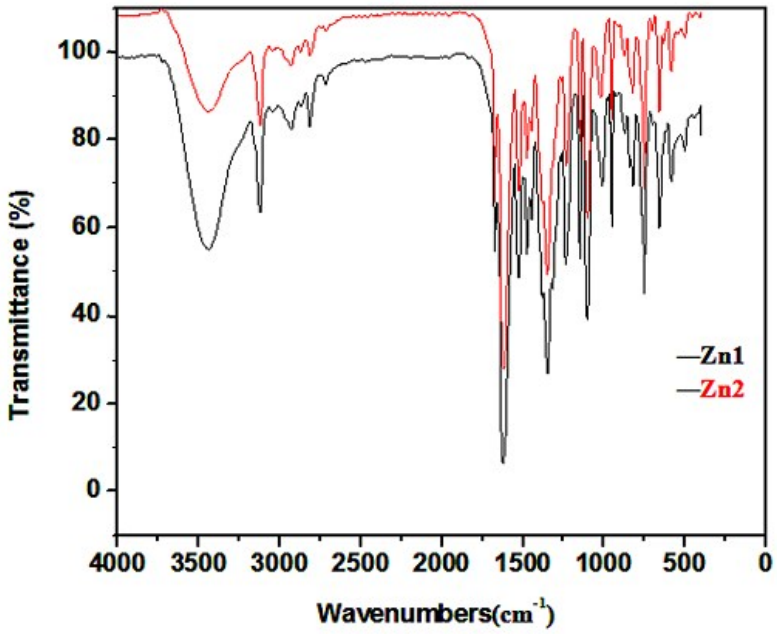

Figure S13. IR spectra of complex **1** (black) and soaked **1** in $CHCl_3$ solution (red)

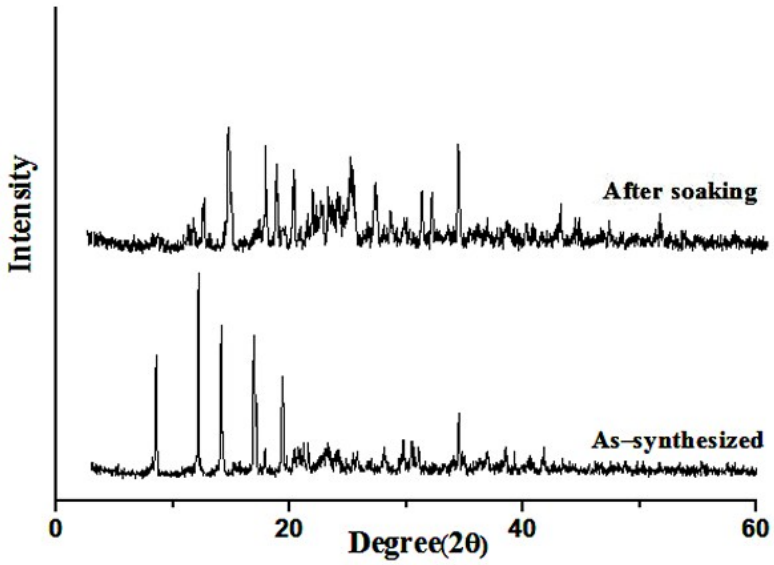

Figure S14. Powder X-ray diffraction patterns of soaked complex **1** in $CHCl_3$ solution

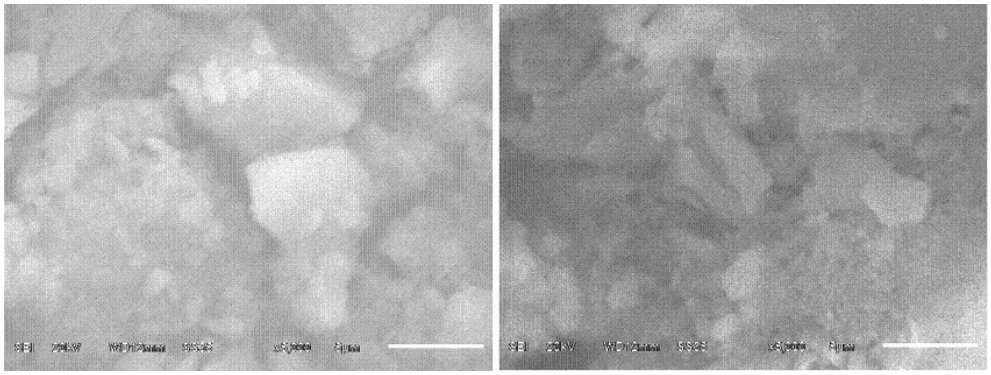

Figure S15. SEM analysis for complex **1**(left) and soaked complex **1** in 0.1 mmol/L C_{60} $CHCl_3$ solution (right)

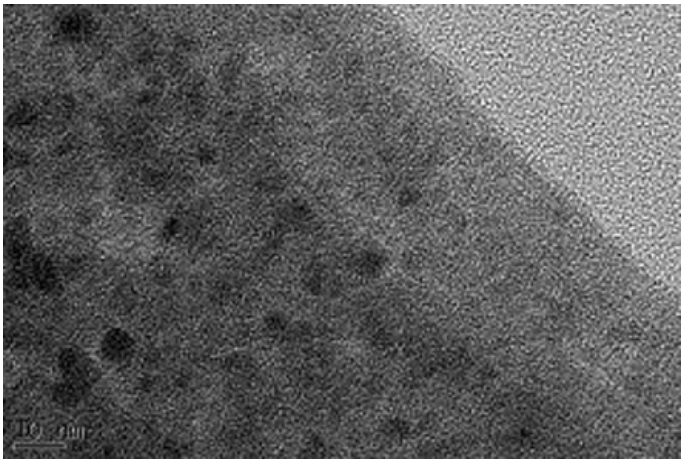

Figure S16. TEM (10 nm) analysis for soaked complex **1**

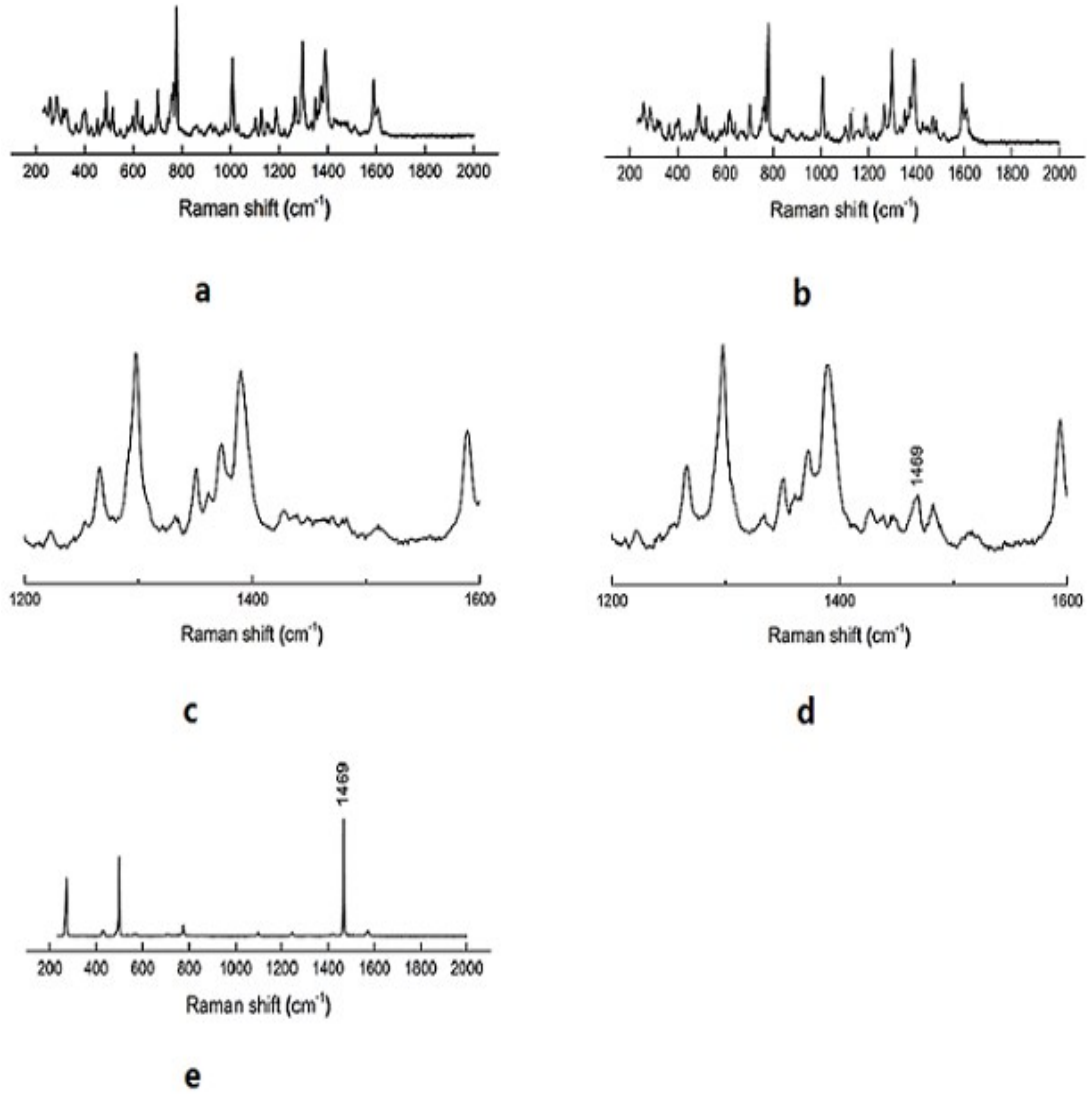

Figure S17. Raman spectra of complex **1** (a), complex **1** soaked in C_{60} $CHCl_3$ solution (b), local enlargement of a (c), local enlargement of b (d), C_{60} (e).

Table S1. Selected bond lengths (Å) and angles (deg) for **1** , **2** and **3**.

Compound 1			
Zn1—O1	1.956 (2)	Zn1—O4	1.973 (3)
Zn1—N3	2.012 (3)	Zn1—N1	2.029 (3)
O1—Zn1—O4	102.04 (11)	O1—Zn1—N3	120.25 (11)
O4—Zn1—N3	110.95 (11)	O1—Zn1—N1	100.57 (11)
O4—Zn1—N1	118.11 (10)	N3—Zn1—N1	105.29 (11)
C17—O1—Zn1	124.4 (2)	C1—N1—Zn1	129.7 (2)
C3—N1—Zn1	124.2 (2)	C15—N3—Zn1	126.1 (2)
C16—N3—Zn1	127.7 (2)		
Compound 2			
Cd1—N4	2.244 (5)	Cd1—N1	2.244 (4)
Cd1—O2	2.414 (4)	Cd1—O4	2.445 (4)

Cd1—O5	2.514 (5)	Cd1—O3	2.582 (5)
Cd1—O4^{i}	2.613 (4)	O4—Cd1^{i}	2.613 (4)
N4—Cd1—N1	167.18 (19)	N4—Cd1—O2	90.4 (2)
N1—Cd1—O2	95.1 (2)	N4—Cd1—O4	94.85 (19)
N1—Cd1—O4	88.07 (18)	O2—Cd1—O4	141.56 (14)
N4—Cd1—O5	91.1 (2)	N1—Cd1—O5	100.53 (19)
O2—Cd1—O5	89.13 (14)	O4—Cd1—O5	52.78 (14)
N4—Cd1—O3	88.7 (2)	N1—Cd1—O3	85.67 (19)
O2—Cd1—O3	51.49 (14)	O4—Cd1—O3	166.22 (15)
O5—Cd1—O3	140.61 (14)	N4—Cd1—O4^{i}	82.72 (18)
N1—Cd1—O4^{i}	85.83 (18)	O2—Cd1—O4^{i}	141.80 (14)
O4—Cd1—O4^{i}	76.61 (14)	O5—Cd1—O4^{i}	128.35 (14)
O3—Cd1—O4^{i}	90.68 (13)	C3—N1—Cd1	124.6 (4)
C1—N1—Cd1	130.3 (4)	C15—N4—Cd1	125.8 (5)
C16—N4—Cd1	129.2 (5)	C18—O2—Cd1	97.5 (3)
C18—O3—Cd1	90.2 (3)	C25—O4—Cd1	94.2 (3)
C25—O4—Cd1^{i}	157.6 (4)	Cd1—O4—Cd1^{i}	103.08 (14)
C25—O5—Cd1	91.9 (3)		

Symmetric codes: i=x, −y+2, −z+1.

Compound 3

N1—Co1	2.035(4)	O1—Co1	1.988(4)
N5—Co3^{i}	2.006(4)	O4—Co3	1.979(4)
N6—Co3^{ii}	2.031(4)	O7—Co2	1.968(4)
N8—Co1^{iii}	2.016(5)	O10—Co2^{vi}	1.980(3)
N9—Co2	1.998(5)	O11—Co1	1.962(4)
N12—Co2^{iv}	2.003(5)	O15—Co3^{vii}	1.973(4)
N15—Co4	2.015(5)	O20—Co4	1.985(4)
N16—Co4^{v}	2.025(4)	O24—Co4^{viii}	1.968(3)
Co1—N8^{iii}	2.016(5)	Co2—N12^{iv}	2.003(5)
Co2—O10^{viii}	1.980(3)	Co3—O15^{ix}	1.973(4)
Co3—N5^{x}	2.006(4)	Co3—N6^{ii}	2.031(4)
Co4—O24^{vi}	1.968(3)	Co4—N16^{v}	2.025(4)
C66—N5—Co3^{i}	125.0(4)	C71—N6—Co3^{ii}	123.2(3)
C68—N5—Co3^{i}	128.9(4)	C75—N8—Co1^{iii}	130.4(5)
C69—N6—Co3^{ii}	130.2(4)	C89—N12—Co2^{iv}	123.6(4)
C74—N8—Co1^{iii}	122.8(4)	C91—N12—Co2^{iv}	130.0(4)
C108—N16—Co4^{v}	123.8(4)	C105—N15—Co4	130.6(4)
C109—N16—Co4^{v}	130.4(4)	C106—N15—Co4	125.5(3)
C1—O1—Co1	101.4(3)	C19—O8—C22	117.5(4)
C14—O4—Co3	114.3(3)	C28—O10—Co2^{vi}	111.2(3)
C15—O7—Co2	107.1(3)	C29—O11—Co1	115.8(4)
C42—O15—Co3^{vii}	106.1(4)	O11—Co1—O1	107.22(15)
C110—O20—Co4	104.0(3)	O11—Co1—N8^{iii}	108.21(18)
C123—O24—Co4^{viii}	121.8(3)	O1—Co1—N8^{iii}	127.28(18)

O11—Co1—N1	94.50(17)	O1—Co1—N1	113.73(16)
N8^{iii}—Co1—N1	100.99(18)	O7—Co2—N12^{iv}	120.87(16)
O7—Co2—O10^{viii}	112.22(15)	O10^{viii}—Co2—N12^{iv}	108.59(16)
O7—Co2—N9	114.51(17)	N9—Co2—N12^{iv}	103.11(19)
O10^{viii}—Co2—N9	93.96(16)	O15^{ix}—Co3—O4	107.55(16)
O15^{ix}—Co3—N5^{x}	116.58(18)	O24^{vi}—Co4—O20	103.87(16)
O4—Co3—N6^{ii}	95.23(17)	O24^{vi}—Co4—N15	94.05(16)
N5^{x}—Co3—N6^{ii}	109.38(18)	O20—Co4—N15	114.68(17)
O24^{vi}—Co4—N16^{v}	112.79(16)	N15—Co4—N16^{v}	106.00(18)
O20—Co4—N16^{v}	122.02(16)		

Symmetric codes: i) x, -1+y, z; (ii) -1-x, 2-y, 1-z; (iii) -x, 2-y, 1-z; (iv) 1-x, 1-y, 2-z; (v) -x, -y, 2-z; (vi) 1+x, y, z; (vii) 1+x, -1+y, z; (viii) -1+x, y, z; (ix) -1+x, 1+y, z; (x) x, 1+y, z.