Electronic Supplementary Material (ESI) for RSC Advances.

A Series of Multidimensional MOFs Incorporating a new N-heterocyclic Building Block: 5,5'-di(pyridin-4-yl)-3,3'-bi(1,2,4-triazole)

Peng-Fei Yao,[a] Hai-Ye Li,[a] Fu-Ping Huang,*[a] Qing Yu,[a] Xao-Huan Qin,[a] Jie Tang,[a] Ye Tao[a], He-Dong Bian*[b]

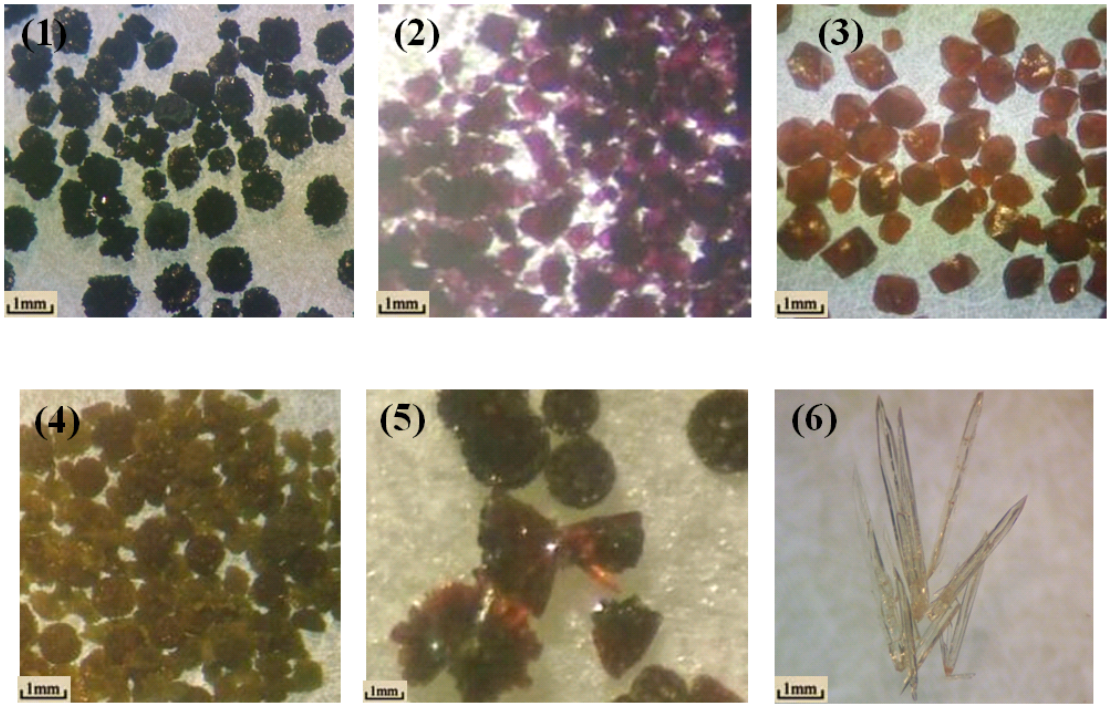


Fig **S1** The crystal morphology of **1**- **6**.

Table S1 Selected bond lengths (Å) and angles (º) for **1**–**6**.

1 (Symmetry codes: (A) *x*, *y*, *z*+1; (B) *x*+1, *y*, *z*; (C) −*x*+1, −*y*+1, −*z*+1.)

*[a] Key Laboratory for the Chemistry and Molecular Engineering of Medicinal Resources (Ministry of Education of China), School of Chemistry and Pharmacy, Guangxi Normal University, Guilin, 541004, P. R. China. E-mail: huangfp2010@163.com

*[b] School of Chemistry and Chemical Engineering, Guangxi University for Nationalities, Key Laboratory of Chemistry and Engineering of Forest Products, Nanning, 530008, P. R. China. E-mail: gxunchem@163.com

Co1—Cl1	2.2122 (19)	Co2—Cl3	2.6446 (17)	Co3—Cl3	2.2541 (17)
Co1—Cl2	2.229 (2)	Co2—N4	1.941 (4)	Co3—Cl4	2.219 (2)
Co1—N3	2.034 (4)	Co2—N5	1.941 (4)	Co3—N1A	2.031 (4)
Co1—N6C	2.030 (4)	N4—Co2—Cl3	89.85 (14)	Co3—N8B	2.015 (4)
Cl1—Co1—Cl2	118.35 (9)	N4—Co2—Cl3C	90.15 (14)	Cl4—Co3—Cl3	106.49 (7)
N3—Co1—Cl1	107.61 (13)	N4C—Co2—Cl3C	89.85 (14)	N1A—Co3—Cl3	108.31 (14)
N3—Co1—Cl2	105.56 (14)	N5—Co2—Cl3	87.48 (14)	N1A—Co3—Cl4	107.51 (15)
N6C—Co1—Cl1	109.75 (14)	N5—Co2—Cl3C	92.52 (14)	N8B—Co3—Cl3	109.58 (14)
N6C—Co1—Cl2	107.69 (14)	N5—Co2—N4C	98.98 (17)	N8B—Co3—Cl4	112.52 (16)
N6C—Co1—N3	107.33 (16)	N5—Co2—N4	81.02 (17)	N8B—Co3—N1A	112.18 (19)

2 (Symmetry codes: (A) −*x*+1, −*y*+1, −*z*+1; (B) −*x*, −*y*+1, −*z*+1; (C) *x*+1, *y*, *z*; (D) −*x*, −*y*, −*z*+1.)

Co1—O1	2.116 (3)	Co2—O2	1.945 (4)	Co2—N1	2.191 (4)
Co1—O3	2.118 (4)	Co2—O4	1.953 (4)	Co2—N2B	2.191 (4)
Co1—N3B	2.106 (4)	N3C—Co1—O3	88.68 (15)	Co2—N4D	2.114 (4)
O1—Co1—O3A	86.48 (15)	O2—Co2—O4	126.5 (2)	O4—Co2—N2B	92.35 (16)
O1—Co1—O3	93.52 (16)	O2—Co2—N1	111.89 (18)	O4—Co2—N4D	92.12 (17)
N3B—Co1—O1	89.32 (15)	O2—Co2—N2B	91.11 (17)	N2B—Co2—N1	80.33 (15)
N3C—Co1—O1	90.68 (15)	O2—Co2—N4D	89.54 (17)	N4D—Co2—N1	93.82 (16)
N3B—Co1—O3	91.32 (15)	O4—Co2—N1	121.35 (19)	N4D—Co2—N2B	173.92 (16)

3 and 4 (Symmetry codes: (A) −*x*+1, −*y*, −*z*+2; (B) *x*+1/2, −*y*−1/2, *z*−1/2; (C) −*x*+1/2, *y*+1/2, −*z*+5/2.)

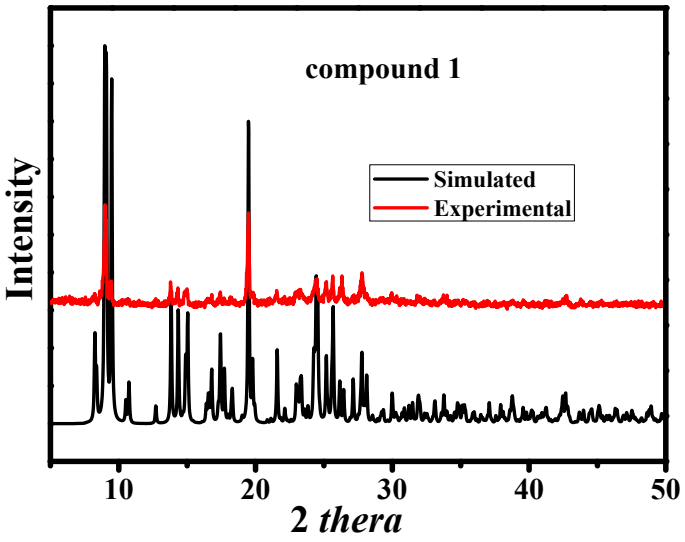
Co1—N4	2.2352 (18)	Co1—N5	2.1188 (18)	Co1—N8B	2.1832 (18)
N5A—Co1—N4	103.54 (7)	N5A—Co1—N8C	90.01 (7)	N8B—Co1—N4A	88.67 (7)
N5—Co1—N4	76.46 (7)	N5—Co1—N8C	89.99 (7)	N8B—Co1—N4	91.33 (7)
Ni1—N4	2.185 (2)	Ni1—N5	2.092 (3)	Ni1—N8B	2.145 (3)
N5—Ni1—N4	77.68 (10)	N5—Ni1—N8C	89.87 (10)	N8B—Ni1—N4	89.02 (9)
N5A—Ni1—N4	102.32 (10)	N5A—Ni1—N8C	90.13 (10)	N8B—Ni1—N4A	90.98 (9)

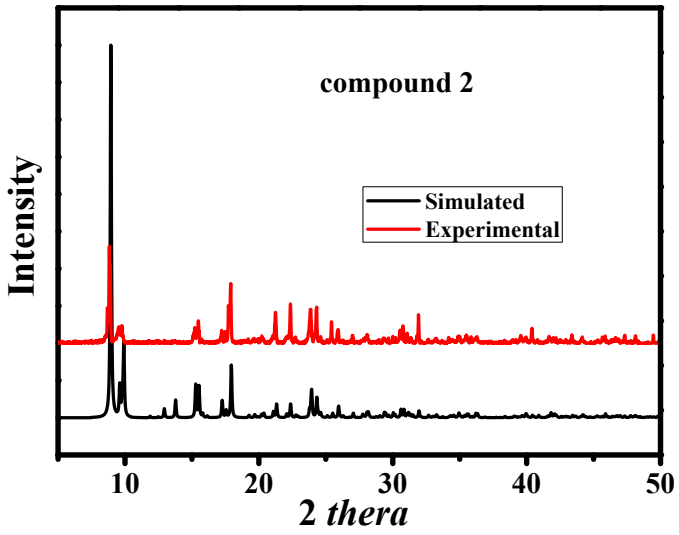
5 (Symmetry codes: (A) −*x*, *y*, −*z*+1/2; (B) −*x*+1/2, *y*−1/2, *z*; (C) *x*−1/2, *y*−1/2, −*z*+1/2; (D) −*x*+1, *y*, −*z*+3/2; (E) *x*, −*y*+1, *z*+1/2; (F) *x*−1/2, *y*−1/2, −*z*+3/2.)

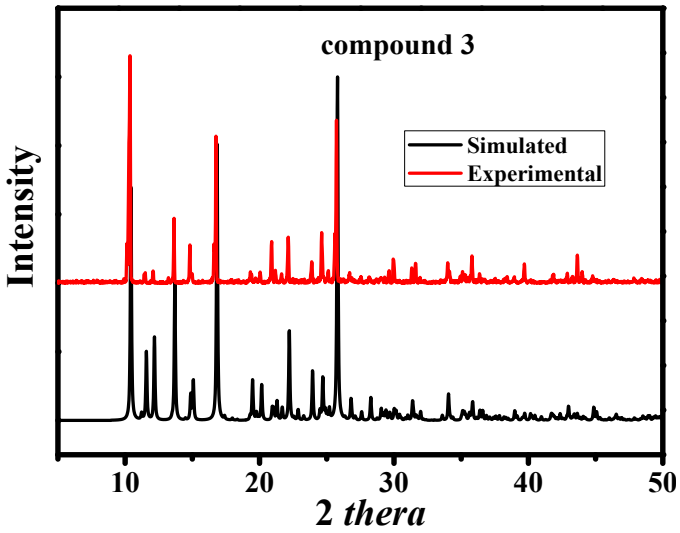
Cu1—N1	2.123 (4)	Cu1—N7B	2.082 (4)	Cu2—N4	1.891 (4)
Cu3—N3	1.967 (3)	Cu3—N6E	2.033 (4)	Cu3—N8F	2.074 (4)
N1—Cu1—N1A	99.3 (2)	N7C—Cu1—N7B	96.58 (19)	N3—Cu3—N8F	129.10 (16)
N7C—Cu1—N1	134.85 (15)	N4—Cu2—N4D	172.5 (2)	N6E—Cu3—N8F	99.76 (16)
N7B—Cu1—N1	99.00 (14)	N3—Cu3—N6E	130.99 (15)		

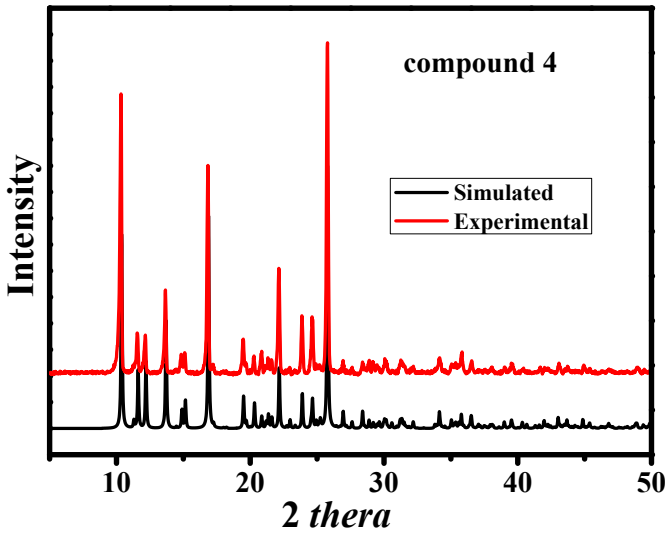
6 (Symmetry codes: (A) −*x*+1/2, *y*, −*z*; (B) −*y*+1/4, −*x*+1/4, −*z*+1/4; (C) *y*+1/4, −*x*+1/4, *z*−1/4.)

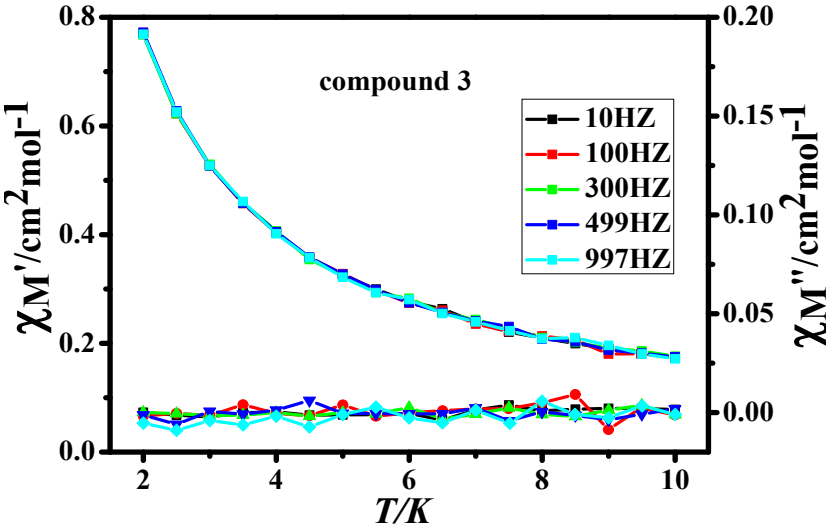
Mn1—O1	2.150 (2)	Mn1—N1	2.3001 (18)	Mn1—N3B	2.3972 (19)
O1—Mn1—O1A	97.27 (12)	O1—Mn1—N3B	88.09 (7)	N1—Mn1—N3B	75.31 (6)
O1—Mn1—N1A	86.69 (7)	O1—Mn1—N3C	161.31 (6)	N1—Mn1—N3C	107.48 (7)
O1—Mn1—N1	90.75 (7)	N1A—Mn1—N1	176.13 (10)	N3B—Mn1—N3C	92.51 (9)

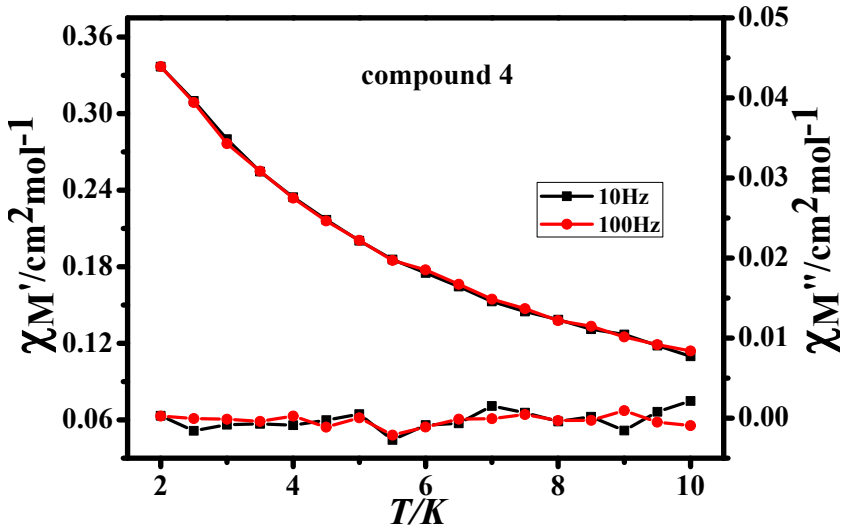

compound 1
Simulated
Experimental
Intensity
10
20
30
40
50
2 thera


compound 2
Simulated
Experimental
Intensity
10
20
30
40
50
2 thera


compound 3
Simulated
Experimental
Intensity
10
20
30
40
50
2 thera


compound 4
Simulated
Experimental
Intensity
10
20
30
40
50
2 thera


compound 3
10HZ
100HZ
300HZ
499HZ
997HZ
χM'/cm2mol-1
χM''/cm2mol-1
0.0
0.2
0.4
0.6
0.8
0.00
0.05
0.10
0.15
0.20
2
4
6
8
10
T/K


compound 4
10Hz
100Hz
χM'/cm2mol-1
χM''/cm2mol-1
0.06
0.12
0.18
0.24
0.30
0.36
0.00
0.01
0.02
0.03
0.04
0.05
2
4
6
8
10
T/K

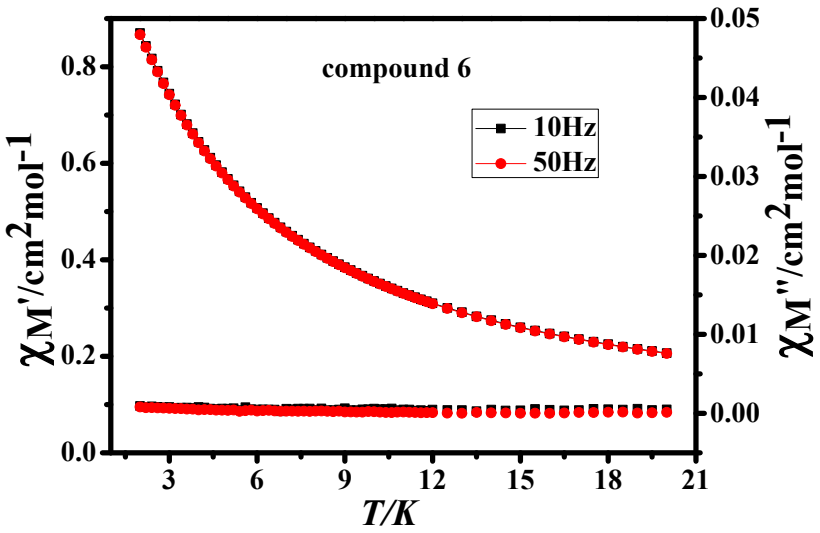


Fig **S3** The in-phase and out-of-phase ac magnetic susceptibilities for **3**, **4** and **6**.