

Supporting Information

Copper-based energetic MOFs with 3-nitro-1*H*-1,2,4-triazole: solvent-depended syntheses, structures and energetic performances

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Table S1. Selected bond lengths (Å) and bond angles (°) for compounds **1-3**.

Compound 1			
N(2)-Cu(1)#1	1.966(4)	C(14)-N(1)-Cu(1)#2	133.3(3)
N(1)-Cu(1)#2	1.938(4)	N(2)-N(1)-Cu(1)#2	123.0(3)
Cu(1)-N(1)#3	1.938(4)	N(1)#3-Cu(1)-N(2)#4	128.34(14)
Cu(1)-N(2)#4	1.966(4)	N(1)#3-Cu(1)-N(3)	121.52(14)
Cu(1)-N(3)	2.032(3)	N(2)#4-Cu(1)-N(3)	110.11(14)
C(8)-N(2)-Cu(1)#1	127.8(3)	C(14)-N(3)-Cu(1)	131.8(3)
N(1)-N(2)-Cu(1)#1	125.1(3)	C(8)-N(3)-Cu(1)	127.3(3)
Symmetry transformations used to generate equivalent atoms:			
#1 -x,y+1/2,-z+3/2	#2 -x+1/2,-y+2,z+1/2	#3 -x+1/2,-y+2,z-1/2	#4 -x,y-1/2,-z+3/2
Compound 2			
Cu(1)-N(5)	1.964(5)	N(5)-Cu(1)-N(5)#1	105.1(2)
Cu(1)-N(1)	1.993(5)	N(1)-Cu(1)-N(5)#1	82.66(19)
Cu(1)-O(3)	2.018(5)	O(3)-Cu(1)-N(5)#1	95.0(2)
Cu(1)-N(2)	2.033(5)	N(2)-Cu(1)-N(5)#1	99.8(2)
Cu(1)-N(5)#1	2.282(5)	C(3)-O(3)-Cu(1)	124.6(5)
N(5)-Cu(1)#2	2.282(5)	C(2)#1-N(1)-Cu(1)	130.8(4)
N(5)-Cu(1)-N(1)	172.0(2)	N(2)#1-N(1)-Cu(1)	125.7(4)
N(5)-Cu(1)-O(3)	90.8(2)	C(1)-N(2)-Cu(1)	131.7(5)
N(1)-Cu(1)-O(3)	90.4(2)	N(1)#2-N(2)-Cu(1)	122.6(4)
N(5)-Cu(1)-N(2)	88.2(2)	N(6)-N(5)-Cu(1)	123.0(4)
N(1)-Cu(1)-N(2)	88.6(2)	N(6)-N(5)-Cu(1)#2	119.6(4)

O(3)-Cu(1)-N(2)	164.9(2)	Cu(1)-N(5)-Cu(1)#2	117.3(2)
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Symmetry transformations used to generate equivalent atoms:

#1 $x, -y+1/2, z+1/2$	#2 $x, -y+1/2, z-1/2$
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Compound 3

Cu(1)-N(5)	1.938(4)	N(5)-Cu(1)-N(5)#2	106.91(14)
Cu(1)-N(1)	1.977(4)	N(1)-Cu(1)-N(5)#2	83.48(15)

Cu(1)-N(2)#1	2.038(4)	N(2)#1-Cu(1)-N(5)#2	102.50(15)
Cu(1)-O(1)	2.081(3)	O(1)-Cu(1)-N(5)#2	86.68(14)
Cu(1)-N(5)#2	2.226(4)	Cu(1)-O(1)-H(1A)	111.0
N(2)-Cu(1)#2	2.038(4)	Cu(1)-O(1)-H(1B)	110.3
N(5)-Cu(1)#1	2.226(4)	C(1)-N(2)-Cu(1)#2	131.6(4)
N(5)-Cu(1)-N(1)	169.54(16)	N(1)-N(2)-Cu(1)#2	122.7(3)
N(5)-Cu(1)-N(2)#1	87.35(16)	C(2)-N(1)-Cu(1)	131.6(3)
N(1)-Cu(1)-N(2)#1	89.21(15)	N(2)-N(1)-Cu(1)	124.0(3)
N(5)-Cu(1)-O(1)	91.45(14)	N(6)-N(5)-Cu(1)	122.4(3)
N(1)-Cu(1)-O(1)	90.36(14)	N(6)-N(5)-Cu(1)#1	118.8(3)
N(2)#1-Cu(1)-O(1)	170.70(14)	Cu(1)-N(5)-Cu(1)#1	118.44(18)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1/2, y-1/2, z$	#2 $-x+1/2, y+1/2, z$
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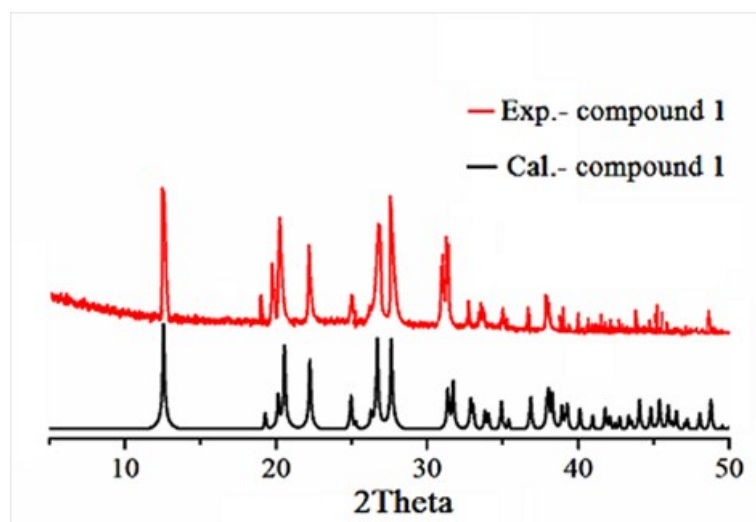


Fig. S1. XRPD curves for compound 1.

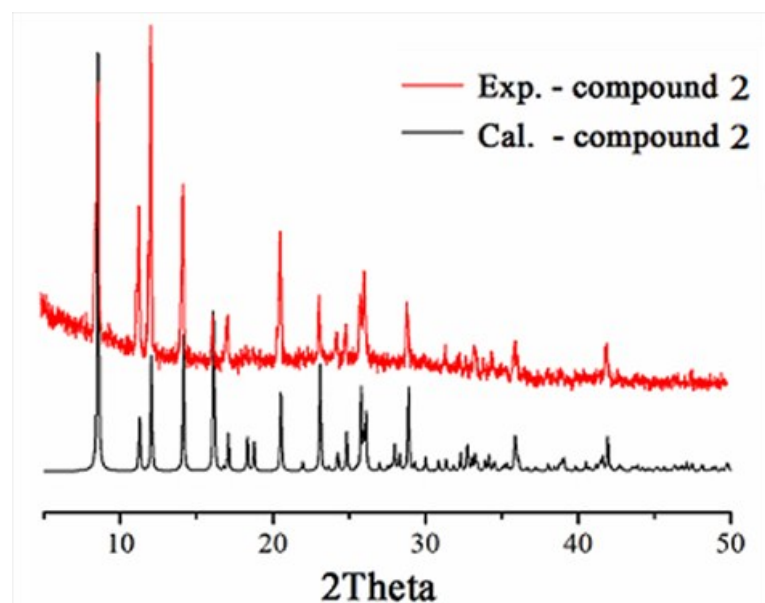


Fig. S2. XRPD curves for compound 2.

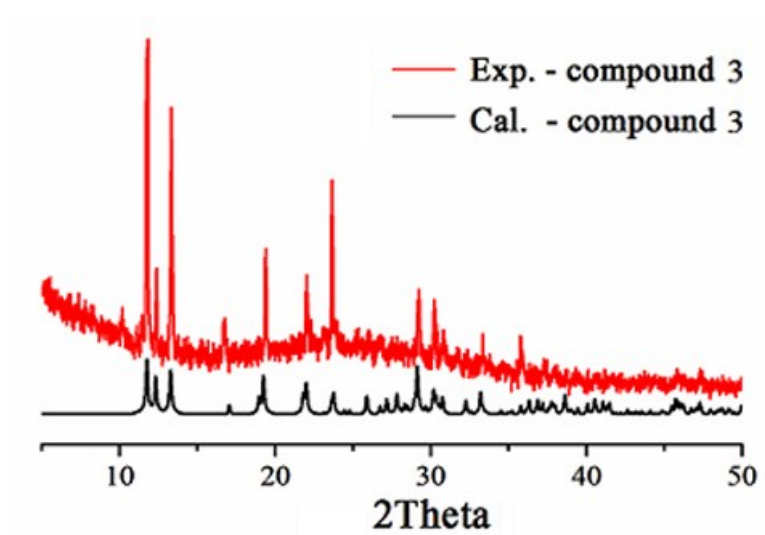


Fig. S3. XRPD curves for compound 3.