

Controllable Nitric Oxide Storage and Release in Cu-BTC: Crystallographic Insights and Bioactivity

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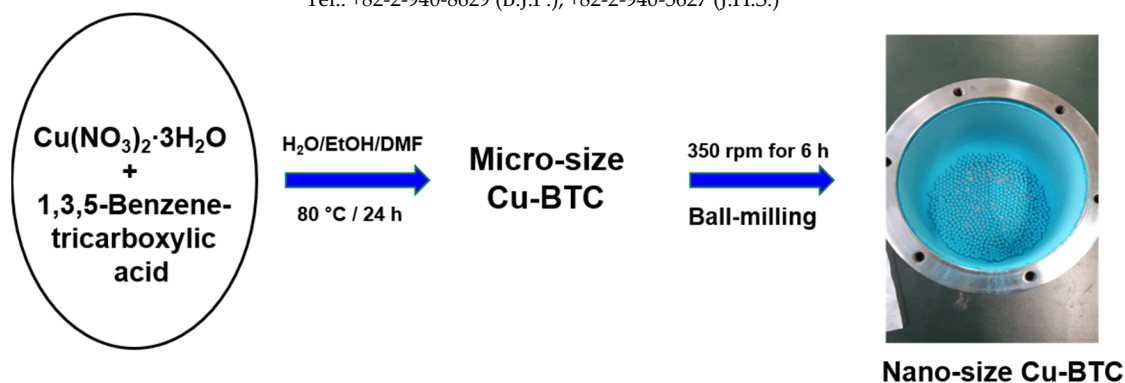


Figure S1. Schematic of the synthesis of micro-sized Cu-BTC (1, BTC: benzene-1,3,5-tricarboxylate) by a solvothermal reaction and the preparation of nano-sized Cu-BTC (2) by ball milling.

Table S1. Bond lengths [Å] and angles [°] for NO \subset Cu-BTC (NO: nitric oxide).

Cu(1)-O(1)	1.951(4)
Cu(1)-O(1)#1	1.951(4)
Cu(1)-O(1)#2	1.951(4)
Cu(1)-O(1)#3	1.951(4)
Cu(1)-O(2)	2.192(11)
Cu(1)-Cu(1)#4	2.622(3)
O(1)-C(1)	1.260(5)
C(1)-O(1)#5	1.260(5)
C(1)-C(2)	1.492(10)
C(2)-C(3)#6	1.385(6)
C(2)-C(3)	1.385(6)
C(3)-C(2)#7	1.385(6)
C(3)-H(3)	0.9400
N(11)-O(11)	1.150(2)
O(1)-Cu(1)-O(1)#1	89.1(3)
O(1)-Cu(1)-O(1)#2	89.8(3)
O(1)#1-Cu(1)-O(1)#2	168.8(2)
O(1)-Cu(1)-O(1)#3	168.8(2)
O(1)#1-Cu(1)-O(1)#3	89.8(3)
O(1)#2-Cu(1)-O(1)#3	89.1(3)
O(1)-Cu(1)-O(2)	95.59(12)
O(1)#1-Cu(1)-O(2)	95.58(12)
O(1)#2-Cu(1)-O(2)	95.58(12)

O(1)#3-Cu(1)-O(2)	95.58(12)
O(1)-Cu(1)-Cu(1)#4	84.41(12)
O(1)#1-Cu(1)-Cu(1)#4	84.42(12)
O(1)#2-Cu(1)-Cu(1)#4	84.42(12)
O(1)#3-Cu(1)-Cu(1)#4	84.42(12)
O(2)-Cu(1)-Cu(1)#4	180.0(3)
C(1)-O(1)-Cu(1)	122.7(4)
O(1)-C(1)-O(1)#5	125.6(7)
O(1)-C(1)-C(2)	117.2(4)
O(1)#5-C(1)-C(2)	117.2(4)
C(3)#6-C(2)-C(3)	118.6(8)
C(3)#6-C(2)-C(1)	120.6(4)
C(3)-C(2)-C(1)	120.6(4)
C(2)-C(3)-C(2)#7	121.5(8)
C(2)-C(3)-H(3)	119.3
C(2)#7-C(3)-H(3)	119.3

Symmetry transformations used for generating equivalent atoms:

#1 y, x, z ; #2 $x, y, -z+2$; #3 $y, x, -z+2$; #4 $-x+1/2, -y+1/2, -z+2$; #5 $-y+1/2, -x+1/2, z$; #6 $-y+1/2, -z+1, x+1/2$; #7 $z-1/2, -x+1/2, -y+1$

Table S2. The nitrogen sorption properties of micro-sized Cu-BTC and nano-sized Cu-BTC.

	Micro-sized Cu-BTC	Nano-sized Cu-BTC
Specific surface area ($\text{m}^2 \text{g}^{-1}$)	799	27
Micropore volume ($\text{cm}^3 \text{g}^{-1}$)	0.3283	0.0092
Mesopore volume ($\text{cm}^3 \text{g}^{-1}$)	0.0096	0.0570
Mean pore diameter (nm)	1.5234	9.9172