Supporting Information

A versatile Cu^{II}/Cu^{I} metal-organic framework for selective sorption and heterogeneous catalysis

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Contents

Table S1. Selected bond lengths (Å) and bond angles (º) for **1** and **2**.

			1		
Cu(1)-N(3)		2.089(5)	N(3)-Cu(1)-I(1)		104.76(16)
Cu(1)-I(1)		2.6454(10)	N(3)-Cu(1)-I(2)#1		108.40(15)
Cu(1)-I(2)#1		2.6554(10)	I(1)-Cu(1)-I(2)#1		116.55(3)
Cu(1)-I(2)		2.086(5)	N(3)-Cu(1)-I(2)		103.36(16)
Cu(2)-N(1)		2.080(5)	I(1)-Cu(1)-I(2)		175.9(2)
Cu(2)-I(1)#2		2.134(5)	I(2)#1-Cu(1)-I(2)		115.44(3)
Cu(2)-I(1)#1	Cu(2)-	2.6284(10)	N(1)-Cu(2)-I(1)#2		108.38(17)
I(2)		2.7043(10)	N(1)-Cu(2)-I(1)#1	N(1)-	108.48(16)
Cu(3)-O(1)		1.938(5)	Cu(2)-I(2)		99.96(16)
Cu(3)-O(8)#4	Cu(3)-	1.955(5)	I(1)#2-Cu(2)-I(2)	O(1)-	103.87(3)
N(4)#4		1.983(5)	Cu(3)-O(8)#4		171.1(2)
Cu(3)-N(2)		1.987(5)	O(1)-Cu(3)-N(4)#4	O(8)#4-	94.8(2)
Cu(3)-O(1W)		2.222(6)	Cu(3)-N(4)#4		83.1(2)
O(8)#4-Cu(3)-O(1W)		91.2(2)	O(1)-Cu(3)-N(2)		83.5(2)
N(4)#4-Cu(3)-O(1W)		95.5(2)	O(8)#4-Cu(3)-N(2)		96.5(2)
N(2)-Cu(3)-O(1W)		98.2(2)	N(4)#4-Cu(3)-N(2)		166.3(3)
I(1)#1-Cu(2)-I(2)		114.77(4)	O(1)-Cu(3)-O(1W)		97.6(2)

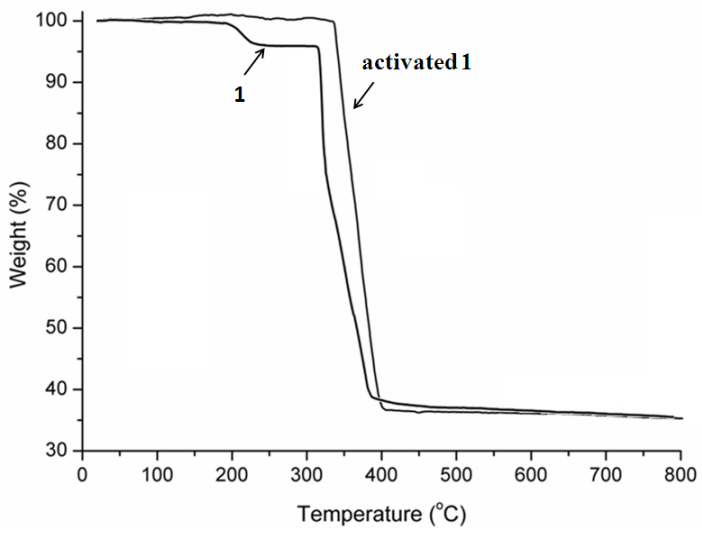

Figure S1. The TG curves of **1** and activated **1**.

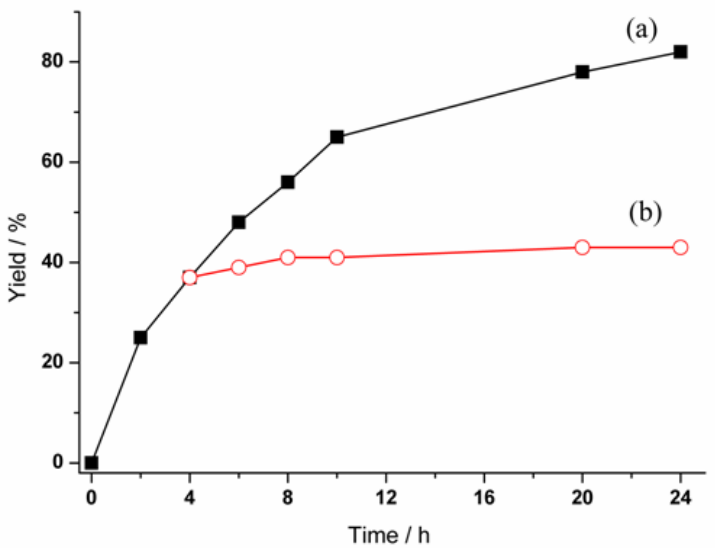

Figure S2. Tertrlin oxidation at 60℃ in MeCN; (a) with a catalyst; (b) filtrate (catalyst filtered off after 4 h of reaction)

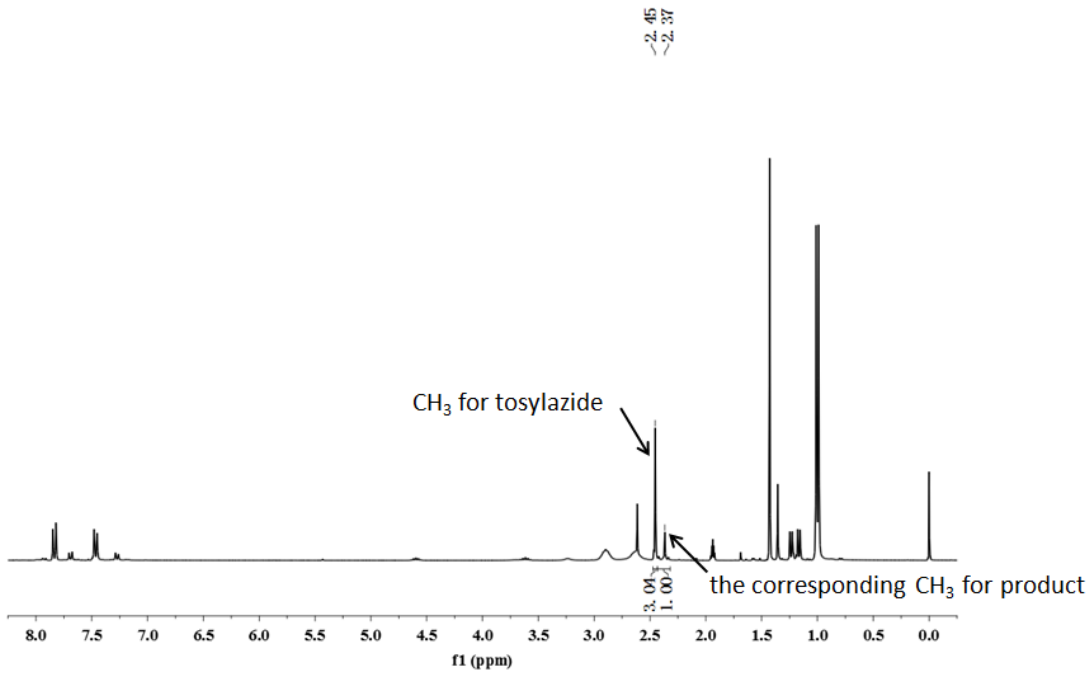

Figure S3. The ^{1}H NMR (300M) spectra of three-component coupling of Ts-N_3, PhCCH and $(i\text{-Pr})_2$NH in the presence of activated Cu^{II}/Cu^{I}-MOF in 1h.

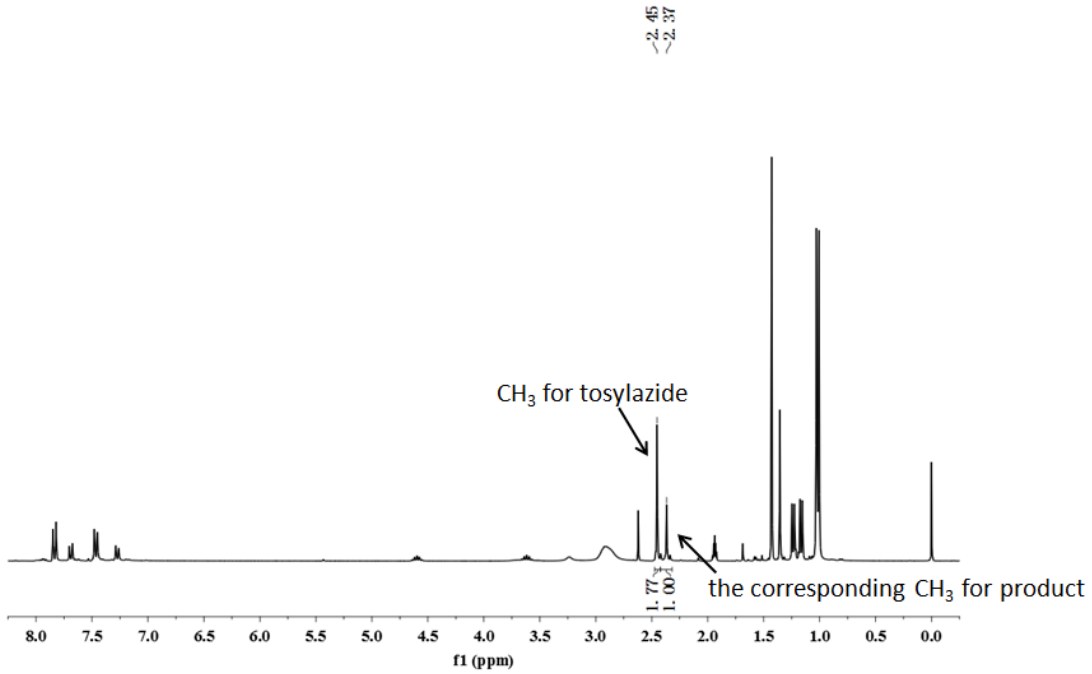

Figure S4 The ^{1}H NMR (300M) spectra of three-component coupling of Ts-N_3, PhCCH and $(i\text{-Pr})_2$NH in the presence of activated Cu^{II}/Cu^{I}-MOF in 2h.

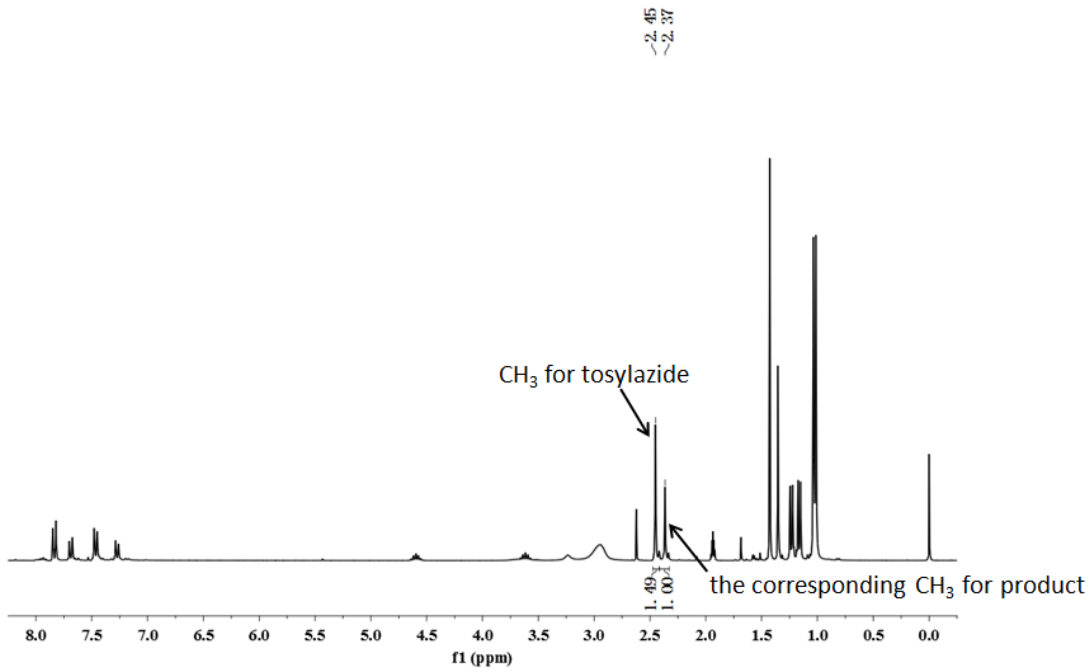

Figure S5. The ^{1}H NMR (300M) spectra of three-component coupling of Ts-N_3, PhCCH and (i-Pr)$_2$NH in the presence of activated Cu^{II}/Cu^{I}-MOF in 3h.