

Supporting Information

for

Accumulation of Versatile Iodine Species by a Porous Hydrogen-Bonding Cu(II) Coordination Framework

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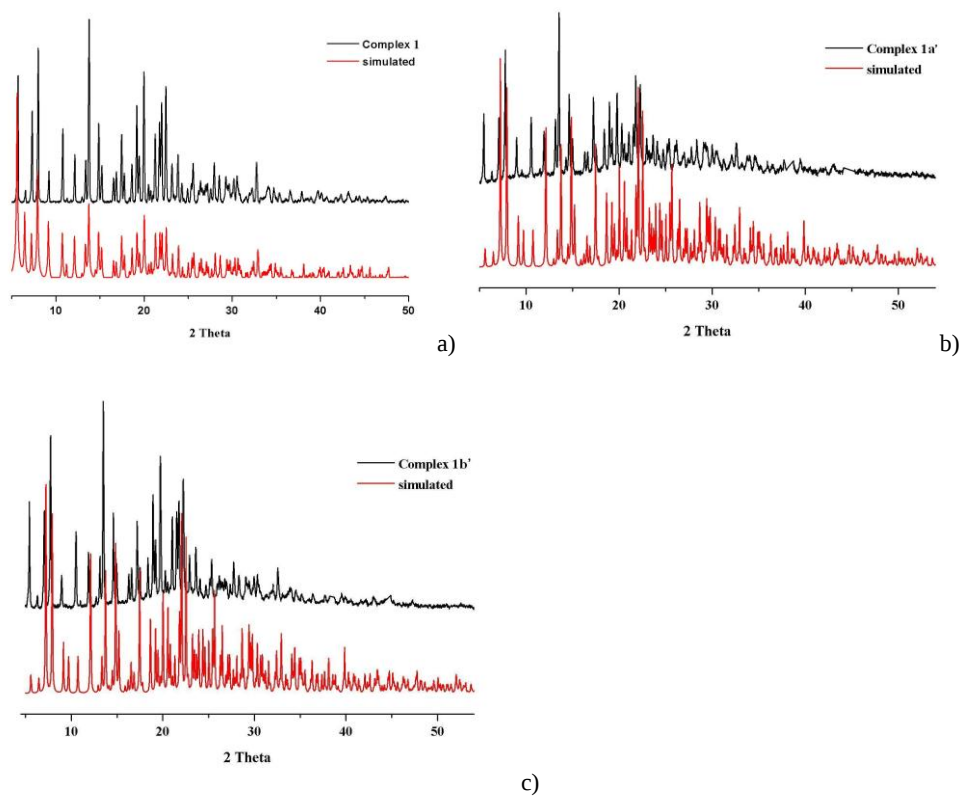


Figure S1. PXRD spectra of compounds **1**(a), **1a'** (b) and **1b'** (c).

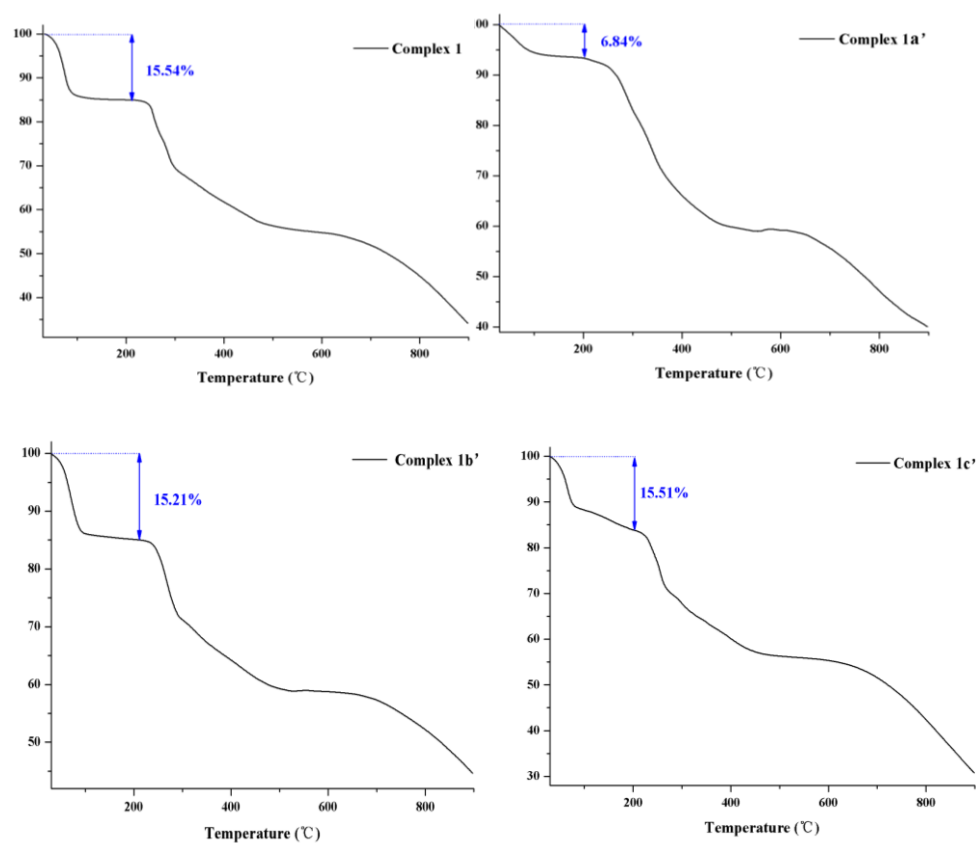


Figure S2. TGA spectra of complexes 1-1c'.

Table S1. Selected bond lengths and angles for complexes **1a-1c**.

Complex 1a		Complex 1b		Complex 1c	
Cu(1)-O(1)	1.952(2)	Cu(1)-O(1)	1.984(10)	Cu(1)-O(1)	1.958(14)
Cu(1)-N(2)	2.031(2)	Cu(1)-N(4)	2.066(12)	Cu(1)-N(3)	2.032(18)
Cu(1)-N(4)	2.054(3)	Cu(1)-N(2)	2.025(14)	Cu(1)-N(5)	2.020(18)
Cu(1)-N(6)	2.118(2)	Cu(1)-N(1)	2.093(13)	Cu(1)-N(1)	2.126(18)
Cu(1)-N(1)	2.126(3)	Cu(1)-N(6)	2.134(11)	Cu(1)-N(6)	2.02(2)
O(1)-Cu(1)-N(2)	101.19(10)	O(1)-Cu(1)-N(4)	103.2(6)	O(1)-Cu(1)-N(3)	95.9(6)
O(1)-Cu(1)-N(4)	102.52(10)	O(1)-Cu(1)-N(2)	99.2(6)	O(1)-Cu(1)-N(1)	173.5(6)
N(2)-Cu(1)-N(4)	124.69(10)	N(4)-Cu(1)-N(2)	125.9(6)	N(5)-Cu(1)-N(6)	125.0(7)
O(1)-Cu(1)-N(6)	95.91(9)	O(1)-Cu(1)-N(1)	175.4(6)	O(1)-Cu(1)-N(5)	100.2(6)
N(2)-Cu(1)-N(6)	112.79(10)	N(4)-Cu(1)-N(1)	80.7(7)	N(5)-Cu(1)-N(3)	111.9(6)
N(4)-Cu(1)-N(6)	113.48(10)	N(2)-Cu(1)-N(1)	80.1(6)	N(6)-Cu(1)-N(3)	112.5(7)
O(1)-Cu(1)-N(1)	175.46(9)	O(1)-Cu(1)-N(6)	96.0(5)	O(1)-Cu(1)-N(6)	105.7(7)
N(2)-Cu(1)-N(1)	79.73(10)	N(4)-Cu(1)-N(6)	115.4(6)	N(5)-Cu(1)-N(1)	79.6(6)
N(4)-Cu(1)-N(1)	80.37(10)	N(2)-Cu(1)-N(6)	110.3(6)	N(6)-Cu(1)-N(1)	79.3(8)
N(6)-Cu(1)-N(1)	79.68(9)	N(1)-Cu(1)-N(6)	80.0(6)	N(1)-Cu(1)-N(3)	78.3(6)