Axial substitution of precursor resulted in two high-energy copper(II) complexes with superior detonation performances

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Contents:

Table S1 Bond lengths for **1** and **2**.

1	Atom	Atom	Length/ Å
	N5	N6	1.307(6)
	N5	Cu1[1]	1.986(4)
	N7	C3	1.338(7)
	N7	Cu1[2]	2.375(5)
	N1	C1	1.4200
	N1	Cu1	1.988(3)
	C2	C3	1.333(6)
	N3	N2	1.4200
	O4	Cu1	1.971(4)
	Cu1	N5[1]	1.986(4)
	Cu1	N4	2.029(4)
	Cu1	N7[3]	2.375(5)
	O1	N8	1.260(7)
[1]1-X,2-Y,2-Z; [2]1-X,-1/2+Y,3/2-Z; [3]1-X,1/2+Y,3/2-Z			
2	N6	N7	1.4200
	N7	C1	1.4200
	C1	C2	1.358(9)
	C1	N4	1.4200
	N4	Cu1	1.917(4)
	Cu1	N4[1]	1.917(4)
	Cu1	N3[1]	1.987(7)
	Cu1	N3	1.987(7)
	Cu1	O1	2.511(8)
	N3	C3	1.318(10)
	O1	C4	1.180(12)
	O2	C4	1.330(13)
[1]-X,1-Y,1-Z			

Table S2 Bond angles for **1** and **2**.

1	Atom	Atom	Atom	Angle/°
	N6	N5	Cu1[1]	122.8(3)
	N4	N5	Cu1[1]	127.1(3)
	C3	N7	Cu1[2]	144.9(4)
	N6	N7	Cu1[2]	110.4(3)
	C2	N1	Cu1	110.76(19)
	C1	N1	Cu1	140.58(19)
	O4	Cu1	N5[1]	93.08(18)
	O4	Cu1	N1	94.47(16)
	N5[1]	Cu1	N1	172.43(16)
	O4	Cu1	N4	161.1(2)

	N5[1]	Cu1	N4	92.56(17)
	N1	Cu1	N4	80.11(16)
	O4	Cu1	N7[3]	87.50(19)
	N5[1]	Cu1	N7[3]	91.77(18)
	N1	Cu1	N7[3]	89.09(16)
	N4	Cu1	N7[3]	110.34(19)
	C3	C2	N1	119.3(3)
	N1	C2	N3	108.0
	O2	N8	O3	120.1(5)
	C2	C3	N4	114.5(5)
	[1]1-X,2-Y,2-Z; [2]1-X,-1/2+Y,3/2-Z; [3]1-X,1/2+Y,3/2-Z			
2	C1	N4	Cu1	113.8(3)
	N5	N4	Cu1	137.8(3)
	N4[1]	Cu1	N4	180.0(7)
	N4[1]	Cu1	N3[1]	81.2(5)
	N4	Cu1	N3[1]	98.8(2)
	N3[1]	Cu1	N3	180.000(2)
	N4[1]	Cu1	O1	93.9(7)
	N3	Cu1	O1	80.8(3)
	C3	N3	Cu1	140.8(6)
	C4	O1	Cu1	133.3(8)
	N6	N5	N4	108.0
	C2	C1	N4	115.3(5)
	N4	C1	N7	108.0
	C3	N3	C2	104.8(7)
	N2	C2	C1	131.3(7)
	[1]-X, 1-Y, 1-Z			

Table S3 Hydrogen bond lengths (Å) and angles (°) for **1** and **2**.

	D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
1	O4	H4B	O1[1]	0.85	1.98	2.804(6)	163.5
	O4	H4A	O1[2]	0.78	1.98	2.755(6)	174.9
	N2	H2	O2[3]	0.86	1.86	2.685(6)	160.0
	[1]-X,2-Y,2-Z; [2]-X,1/2+Y,3/2-Z; [3]+X,+Y,-1+Z						
2	N1	H2	N6[1]	0.86	1.88	2.742(13)	175.3
	N7	H3	O2[2]	0.86	1.88	2.696(8)	158.2
	[1]-1+X, 3/2-Y, 1/2+Z; [2]+X, 3/2-Y, -1/2+Z						

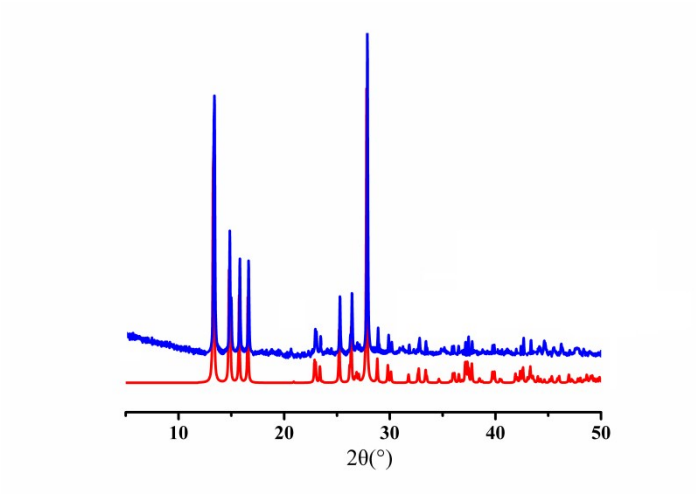

Figure S1 PXRD curve of $[Cu(Htztr)_2(H_2O)_2]_n$ [simulated patterns (red), experimental patterns (blue)].

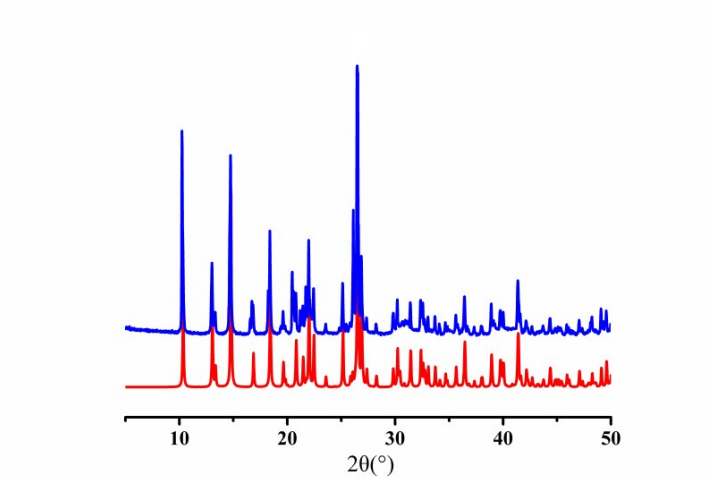

Figure S2 PXRD curve of **1** [simulated patterns (red), experimental patterns (blue)].

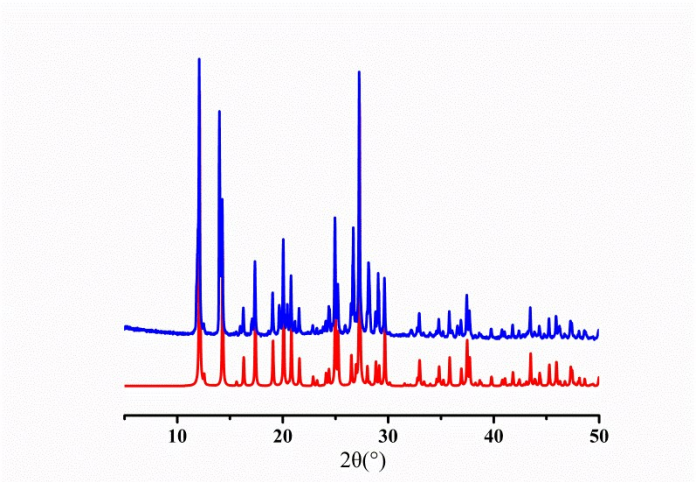

Figure S3 PXRD curve of **2** [simulated patterns (red), experimental patterns (blue)].

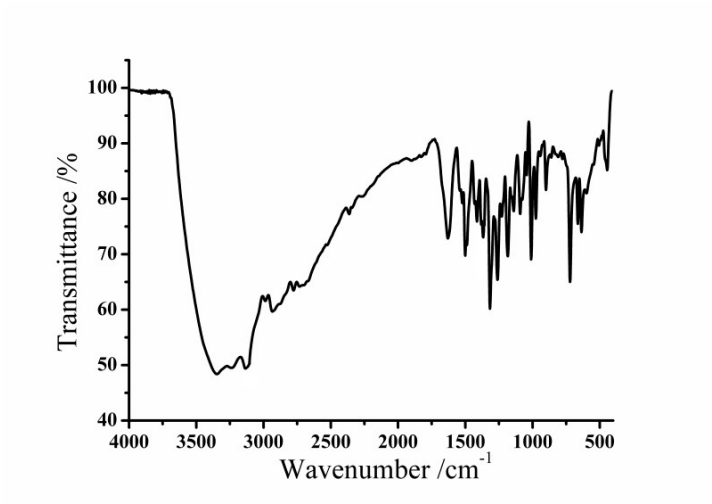

Figure S4 IR spectrum of $[Cu(Htztr)_2(H_2O)_2]_n$

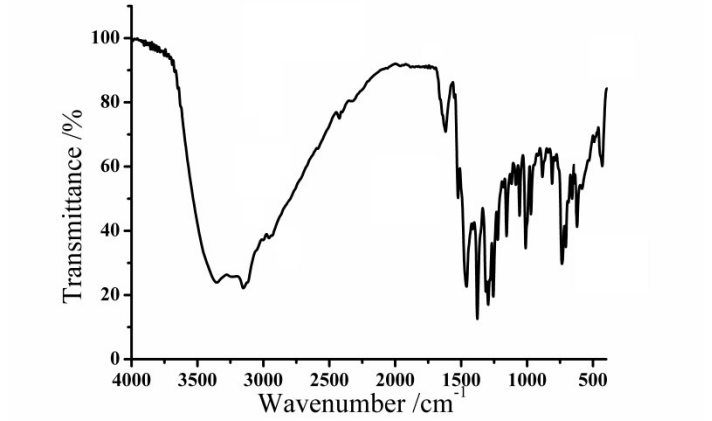

Figure S5 IR spectrum of **1**

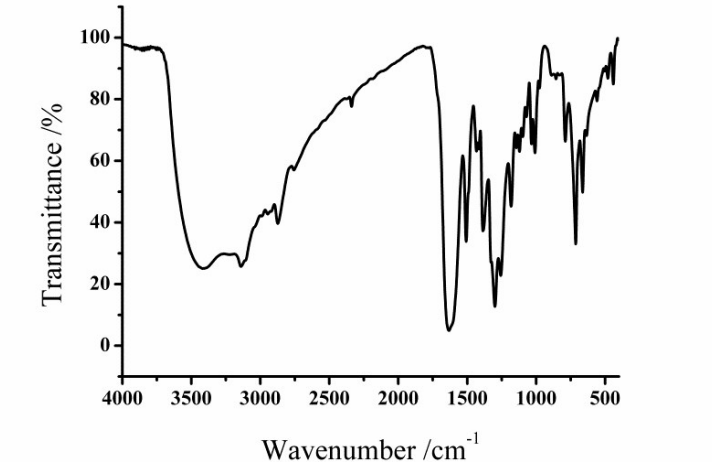

Figure S6 IR spectrum of **2**