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

Xin Li, Qi Yang*, Qing Wei, Gang Xie, Sanping Chen*, ShengliGao

Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an, Shaanxi 710127, China

*E-mail: yangqi@nwu.edu.cn, sanpingchen@126.com

Contents:

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

Table S2 Selected bond angles (°) for 1 and 2.

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

- **Figure S1** PXRD curve of [Cu(Htztr)₂(H₂O)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(H₂O)₂]_n

Figure S5 IR spectrum of 1

Figure S6 IR spectrum of 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	N51	1.986(4)
	Cu1	N4	2.029(4)
	Cu1	N7 ³	2.375(5)
	01	N8	1.260(7)
11 V /	1 V 1 7.21 V 1/21	$V_{2/2} = 7 \cdot 31 = V_{1/2}$	V 2/2 7
·1-A,	2-Y,2-Z; 21-X,-1/2+	$1, 3/2-2, -1-\Lambda, 1/2+$	1,5/2 - Z
2	N6	N7	1.4200
2	N6 N7	N7 C1	1.4200 1.4200
2	N6 N7 C1	N7 C1 C2	1.4200 1.4200 1.358(9)
2	N6 N7 C1 C1	N7 C1 C2 N4	1.4200 1.4200 1.358(9) 1.4200
2	N6 N7 C1 C1 N4	N7 C1 C2 N4 Cu1	1.4200 1.4200 1.358(9) 1.4200 1.917(4)
2	2- Y,2-Z, 21-A,-1/2+ N6 N7 C1 C1 N4 Cu1	N7 C1 C2 N4 Cu1 N4 ¹	1.4200 1.4200 1.358(9) 1.4200 1.917(4) 1.917(4)
2	2- Y,2-Z; -1-A,-1/2+ N6 N7 C1 C1 N4 Cu1 Cu1 Cu1	N7 C1 C2 N4 Cu1 N4 ¹ N3 ¹	1.4200 1.4200 1.358(9) 1.4200 1.917(4) 1.917(4) 1.987(7)
2	2- Y,2-Z, 21-A,-1/2+ N6 N7 C1 C1 C1 N4 Cu1 Cu1 Cu1 Cu1	N7 C1 C2 N4 Cu1 N4 ¹ N3 ¹ N3	1.4200 1.4200 1.358(9) 1.4200 1.917(4) 1.917(4) 1.987(7) 1.987(7)
2	N6 N7 C1 C1 C1 N4 Cu1 Cu1 Cu1 Cu1 Cu1	N7 C1 C2 N4 Cu1 N4 ¹ N3 ¹ N3 O1	1.4200 1.4200 1.358(9) 1.4200 1.917(4) 1.917(4) 1.987(7) 1.987(7) 2.511(8)
2	2- Y, 2-Z, 21-A, -1/2+ N6 N7 C1 C1 C1 N4 Cu1 Cu1 Cu1 Cu1 Cu1 Cu1 N3	N7 C1 C2 N4 Cu1 N4 ¹ N3 ¹ N3 O1 C3	1.4200 1.4200 1.358(9) 1.4200 1.917(4) 1.917(4) 1.987(7) 2.511(8) 1.318(10)
2	N6 N7 C1 C1 C1 N4 Cu1 Cu1 Cu1 Cu1 Cu1 N3 O1	N7 C1 C2 N4 Cu1 N4 ¹ N3 ¹ N3 O1 C3 C4	1.4200 1.4200 1.358(9) 1.4200 1.917(4) 1.917(4) 1.987(7) 2.511(8) 1.318(10) 1.180(12)
2	N6 N7 C1 C1 C1 N4 Cu1 Cu1 Cu1 Cu1 Cu1 Cu1 N3 O1 O2	N7 C1 C2 N4 Cu1 N4 ¹ N3 ¹ N3 O1 C3 C4 C4	1.4200 1.4200 1.358(9) 1.4200 1.917(4) 1.917(4) 1.987(7) 2.511(8) 1.318(10) 1.180(12) 1.330(13)

 $Table \ S1 \ {\rm Bond} \ {\rm lengths} \ {\rm for} \ 1 \ {\rm and} \ 2.$

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)

	N51	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)
	N41	Cu1	N31	81.2(5)
	N4	Cu1	N31	98.8(2)
	N3 ¹	Cu1	N3	180.000(2)
	N41	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	Н	А	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/
1	04	H4B	O11	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	N61	0.86	1.88	2.742(13)	175.3
	2.17	112	Ω^{2}	0.96	1 00	2 606(8)	150 2



Figure S1 PXRD curve of $[Cu(Htztr)_2(H_2O)_2]_n$ [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(H₂O)₂]_n



Figure S5 IR spectrum of 1

