

Supporting Information For

Synthesis and Photoluminescent Properties of Two 2-D and 3-D Iodocuprates Modified by Protonated Ligand†

Jiao Song, Yajie Hou and Yunlong Fu *

Fig. S1 IR Spectra of compounds 1-2.

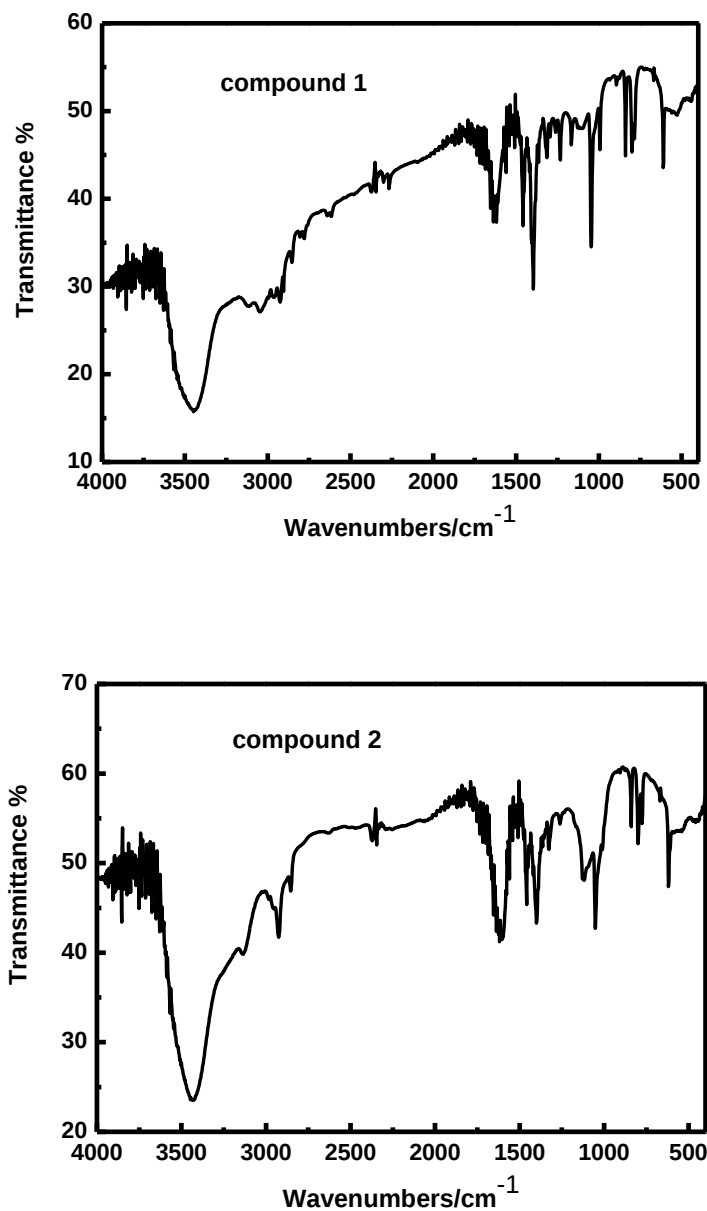


Fig. S2 Experimental and simulated powder XRD patterns of compounds 1- 2.

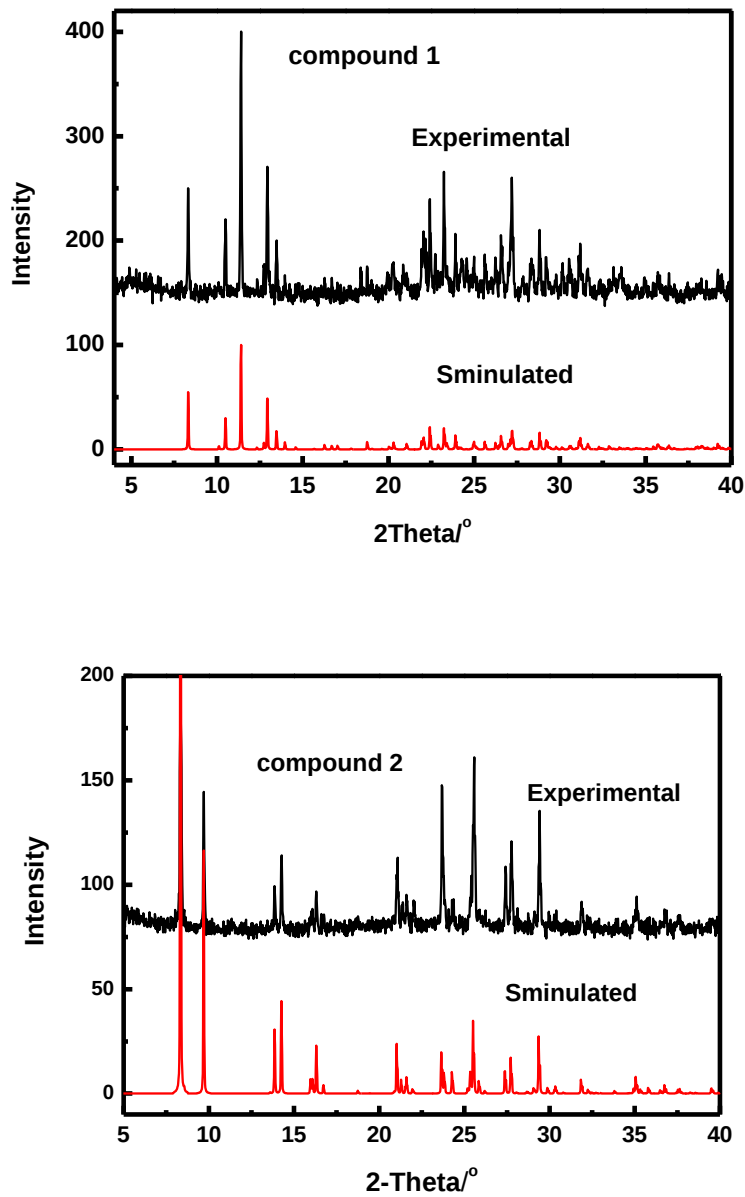


Table S1. Selected bond lengths(Å) and angles (°) for 1- 2^a

1			
I(1)-Cu(2)	2.6431(7)	I(2)-Cu(3)	2.6294(6)
I(1)-Cu(4)	2.6698(7)	I(2)-Cu(2)	2.6473(7)
I(1)-Cu(1)	2.7654(7)	I(2)-Cu(1)	2.7124(7)
I(3)-Cu(2)	2.6685(7)	I(4)-Cu(1)#1	2.6415(7)
I(3)-Cu(4)	2.6968(8)	I(4)-Cu(4)#1	2.6573(7)
I(5)-Cu(3)#2	2.6177(7)	I(4)-Cu(2)	2.7011(7)
I(5)-Cu(1)#2	2.6260(7)	I(5)-Cu(3)	2.7255(7)
Cu(1)-I(5)#2	2.6260(7)	Cu(1)-Cu(2)	2.6838(8)
Cu(1)-I(4)#3	2.6415(7)	Cu(1)-Cu(3)	2.8038(9)

Cu(1)-Cu(4)	2.8361(9)		
Cu(2)-I(1)-Cu(4)	61.69(2)	I(5)#2-Cu(1)-I(4)#3	111.66(2)
Cu(2)-I(1)-Cu(1)	59.449(19)	I(5)#2-Cu(1)-Cu(2)	144.21(3)
Cu(4)-I(1)-Cu(1)	62.88(2)	I(4)#3-Cu(1)-Cu(2)	104.00(3)
Cu(3)-I(2)-Cu(2)	117.69(2)	I(5)#2-Cu(1)-I(2)	113.24(2)
Cu(3)-I(2)-Cu(1)	63.300(19)	I(4)#3-Cu(1)-I(2)	103.81(2)
Cu(2)-I(2)-Cu(1)	60.084(19)	Cu(2)-Cu(1)-I(2)	58.755(19)
Cu(2)-I(3)-Cu(4)	61.02(2)	I(5)#2-Cu(1)-I(1)	104.71(2)
Cu(1)#1-I(4)-Cu(4)#1	64.72(2)	I(4)#3-Cu(1)-I(1)	110.74(2)
Cu(1)#1-I(4)-Cu(2)	134.54(2)	I(2)-Cu(1)-I(1)	112.88(2)
Cu(4)#1-I(4)-Cu(2)	138.71(2)	I(1)-Cu(2)-I(4)	100.91(2)
Cu(3)#2-I(5)-Cu(1)#2	64.649(19)	I(2)-Cu(2)-I(4)	99.97(2)
Cu(3)#2-I(5)-Cu(3)	60.71(2)	I(3)-Cu(2)-I(4)	116.38(2)
Cu(1)#2-I(5)-Cu(3)	109.49(2)	I(1)-Cu(2)-I(3)	112.34(2)
I(1)-Cu(2)-I(2)	119.27(2)	I(2)-Cu(2)-I(3)	107.63(2)
N(3)-Cu(4)-I(4)#3	107.70(12)	N(1)-Cu(3)-I(5)#2	105.66(9)
N(3)-Cu(4)-I(1)	106.25(12)	N(1)-Cu(3)-I(2)	111.98(9)
I(4)#3-Cu(4)-I(1)	113.28(3)	I(5)#2-Cu(3)-I(2)	116.34(2)
N(3)-Cu(4)-I(3)	112.22(13)	N(1)-Cu(3)-I(5)	102.43(9)
I(4)#3-Cu(4)-I(3)	106.83(2)	I(5)#2-Cu(3)-I(5)	119.29(2)
I(1)-Cu(4)-I(3)	110.61(2)	I(2)-Cu(3)-I(5)	100.46(2)
2			
I(1)-Cu(3')	2.625(3)	Cu(1)-N(1)	2.113(10)
I(1)-Cu(3)	2.639(3)	Cu(1)-I(3)#5	2.7579(9)
I(1)-Cu(3')#1	2.640(3)	Cu(1)-I(3)#4	2.7579(9)
I(1)-Cu(3)#2	2.641(3)	Cu(1)-Cu(2)#4	2.9235(15)
I(1)-Cu(2)	2.6929(13)	Cu(1)-Cu(2)#5	2.9235(15)
I(2)-Cu(2)#3	2.6308(12)	Cu(1)-Cu(2)	2.9235(15)
I(2)-Cu(2)	2.6310(12)	Cu(2)-I(3)#5	2.7069(13)
I(3)-Cu(3)#1	2.614(3)	Cu(2)-Cu(3')#1	2.843(3)
I(3)-Cu(3')#1	2.623(3)	Cu(2)-Cu(3)#2	2.876(3)
I(3)-Cu(2)	2.6429(12)	Cu(3)-Cu(3')	1.865(4)
I(3)-Cu(2)#4	2.7069(13)	Cu(3)-Cu(3')#1	1.899(4)
I(3)-Cu(1)	2.7579(9)	Cu(3)-I(3)#2	2.614(3)
I(4)-Cu(3)#5	2.664(3)	Cu(3)-I(1)#1	2.641(3)
I(4)-Cu(3)#4	2.664(3)	Cu(3)-Cu(2)#1	2.876(3)
I(4)-Cu(3)	2.664(3)	Cu(3')-Cu(3)#2	1.899(4)
I(4)-Cu(3)#6	2.664(3)	Cu(3')-I(3)#2	2.623(3)
I(4)-Cu(3)#1	2.664(3)	Cu(3')-I(1)#2	2.640(3)
I(4)-Cu(3)#2	2.664(3)	Cu(3')-Cu(2)#2	2.843(3)
I(4)-Cu(3')#4	2.674(3)	I(4)-Cu(3')#1	2.674(3)
I(4)-Cu(3')#5	2.674(3)	I(4)-Cu(3')#6	2.674(3)
I(4)-Cu(3')#2	2.674(3)	I(4)-Cu(3')	2.674(3)
Cu(3')-I(1)-Cu(3)	41.49(9)	N(1)-Cu(1)-I(3)	108.92(4)

Cu(3')-I(1)-Cu(3')#1	71.38(13)	N(1)-Cu(1)-I(3)#5	108.92(4)
Cu(3)-I(1)-Cu(3')#1	42.17(9)	I(3)-Cu(1)-I(3)#5	110.02(4)
Cu(3')-I(1)-Cu(3)#2	42.28(9)	N(1)-Cu(1)-I(3)#4	108.92(4)
Cu(3)-I(1)-Cu(3)#2	71.13(11)	I(3)-Cu(1)-I(3)#4	110.02(4)
Cu(3')#1-I(1)-Cu(3)#2	72.56(10)	I(3)#5-Cu(1)-I(3)#4	110.02(4)
Cu(3')-I(1)-Cu(2)	102.84(8)	Cu(2)-I(3)-Cu(2)#4	124.04(5)
Cu(3)-I(1)-Cu(2)	102.18(7)	Cu(3)#1-I(3)-Cu(1)	101.67(8)
Cu(3')#1-I(1)-Cu(2)	64.43(7)	Cu(3')#1-I(3)-Cu(1)	101.96(8)
Cu(3)#2-I(1)-Cu(2)	65.25(6)	Cu(2)-I(3)-Cu(1)	65.50(3)
Cu(2)#3-I(2)-Cu(2)	135.88(6)	Cu(2)#4-I(3)-Cu(1)	64.68(3)
Cu(3)#1-I(3)-Cu(3')#1	41.72(9)	Cu(3)#5-I(4)-Cu(3)#4	109.62(5)
Cu(3)#1-I(3)-Cu(2)	102.25(6)	Cu(3)#5-I(4)-Cu(3)	109.62(5)
Cu(3')#1-I(3)-Cu(2)	65.36(7)	Cu(3)#4-I(4)-Cu(3)	109.62(5)
Cu(3)#1-I(3)-Cu(2)#4	65.40(6)	Cu(3)#5-I(4)-Cu(3)#6	70.38(5)
Cu(3')#1-I(3)-Cu(2)#4	102.27(7)	Cu(3)#4-I(4)-Cu(3)#6	70.38(5)
Cu(3)-I(4)-Cu(3)#6	180.00(10)	I(2)-Cu(2)-I(1)	109.21(5)
Cu(3)#5-I(4)-Cu(3)#1	180.00(10)	I(3)-Cu(2)-I(1)	109.85(4)
Cu(3)#4-I(4)-Cu(3)#1	70.38(5)	I(2)-Cu(2)-I(3)#5	103.60(4)
Cu(3)-I(4)-Cu(3)#1	70.38(5)	I(3)-Cu(2)-I(3)#5	115.27(5)
Cu(3)#6-I(4)-Cu(3)#1	109.62(5)	I(1)-Cu(2)-I(3)#5	107.86(4)
Cu(3)#5-I(4)-Cu(3)#2	70.38(5)	Cu(3)#4-I(4)-Cu(3')#5	71.65(9)
Cu(3)#4-I(4)-Cu(3)#2	180.00(10)	Cu(3)-I(4)-Cu(3')#5	138.32(8)
Cu(3)-I(4)-Cu(3)#2	70.38(5)	Cu(3)#6-I(4)-Cu(3')#5	41.68(8)
Cu(3)#6-I(4)-Cu(3)#2	109.62(5)	Cu(3)#1-I(4)-Cu(3')#5	139.11(9)
Cu(3)#1-I(4)-Cu(3)#2	109.62(5)	Cu(3)#2-I(4)-Cu(3')#5	108.35(9)
Cu(3)#5-I(4)-Cu(3')#4	138.32(8)	Cu(3')#4-I(4)-Cu(3')#5	109.89(6)
Cu(3)#4-I(4)-Cu(3')#4	40.89(9)	Cu(3)#5-I(4)-Cu(3')#2	41.68(8)
Cu(3)-I(4)-Cu(3')#4	71.65(9)	Cu(3)#2-I(4)-Cu(3')#4	139.11(9)
Cu(3)#6-I(4)-Cu(3')#4	108.35(9)	Cu(3)#5-I(4)-Cu(3')#5	40.89(9)
Cu(3)#1-I(4)-Cu(3')#4	41.68(8)	I(3)#2-Cu(3)-I(1)	114.19(10)
Cu(3)#4-I(4)-Cu(3')#2	139.11(9)	I(3)#2-Cu(3)-I(1)#1	112.32(9)
Cu(3)-I(4)-Cu(3')#2	108.35(9)	I(1)-Cu(3)-I(1)#1	114.34(9)
Cu(3)#6-I(4)-Cu(3')#2	71.65(9)	Cu(3)#5-I(4)-Cu(3')	71.65(9)
Cu(3)#1-I(4)-Cu(3')#2	138.32(8)	Cu(3)#4-I(4)-Cu(3')	138.32(8)
Cu(3)#2-I(4)-Cu(3')#2	40.89(9)	I(3)#2-Cu(3)-I(4)	105.93(9)
Cu(3')#4-I(4)-Cu(3')#2	180.00(12)	I(1)-Cu(3)-I(4)	104.43(9)
Cu(3')#5-I(4)-Cu(3')#2	70.11(6)	I(1)#1-Cu(3)-I(4)	104.39(10)
Cu(3)-I(4)-Cu(3')	40.89(9)	Cu(3)#6-I(4)-Cu(3')	139.11(9)
Cu(3)#1-I(4)-Cu(3')	108.35(9)	I(3)#2-Cu(3')-I(1)	114.38(12)
Cu(3)#2-I(4)-Cu(3')	41.68(8)	I(3)#2-Cu(3')-I(1)#2	112.16(10)
Cu(3')#4-I(4)-Cu(3')	109.89(6)	I(1)-Cu(3')-I(1)#2	114.83(11)
Cu(3')#5-I(4)-Cu(3')	109.89(6)	I(3)#2-Cu(3')-I(4)	105.42(10)
Cu(3')#2-I(4)-Cu(3')	70.11(6)	I(1)-Cu(3')-I(4)	104.55(10)
Cu(3)#5-I(4)-Cu(3')#1	139.11(9)	I(1)#2-Cu(3')-I(4)	104.14(11)

Cu(3)#4-I(4)-Cu(3')#1	108.35(9)	Cu(3')#4-I(4)-Cu(3')#1	70.11(6)
Cu(3)-I(4)-Cu(3')#1	41.68(8)	Cu(3')#5-I(4)-Cu(3')#1	180.00(12)
Cu(3)#6-I(4)-Cu(3')#1	138.32(8)	Cu(3')#2-I(4)-Cu(3')#1	109.89(6)
Cu(3)#1-I(4)-Cu(3')#1	40.89(9)	Cu(3')-I(4)-Cu(3')#1	70.11(6)
Cu(3)#2-I(4)-Cu(3')#1	71.65(9)	Cu(3)#5-I(4)-Cu(3')#6	108.35(9)
Cu(3)-I(4)-Cu(3')#6	139.11(9)	Cu(3)#4-I(4)-Cu(3')#6	41.68(8)
Cu(3)#6-I(4)-Cu(3')#6	40.89(9)	Cu(3')#5-I(4)-Cu(3')#6	70.11(6)
Cu(3)#1-I(4)-Cu(3')#6	71.65(9)	Cu(3')#2-I(4)-Cu(3')#6	109.89(6)
Cu(3)#2-I(4)-Cu(3')#6	138.32(8)	Cu(3')-I(4)-Cu(3')#6	180.00(12)
Cu(3')#4-I(4)-Cu(3')#6	70.11(6)	Cu(3')#1-I(4)-Cu(3')#6	109.89(6)

^a Symmetry codes: #1 x, -y+1/2, z+1/2; #2 -x+1, -y, -z+1; #3 x, -y+1/2, z-1/2 for **1**; #1 x-y+1, x, -z; #2 y, -x+y+1, -z; #3 -x+4/3, -x+y+2/3, -z+1/6; #4 -y+2, x-y+1, z ; #5 -x+y+1, -x+2, z; #6 -x+2, -y+2, -z; #7 -x+y+1, -x+1, z; #8 -y+1, x-y, z for **2**.

Table S2. Hydrogen bonds(Å) and angles (°) for **1- 2**.

1				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(1)...I(3)#4	0.893(19)	2.74(3)	3.553(4)	152(4)
2				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...N(4)#9	0.91	1.86	2.770(16)	180.0

Symmetry code for **1**: #1 x, -y+1/2, z+1/2; #2 -x+1, -y, -z+1; #3 x, -y+1/2, z-1/2; #4 x-1, -y+1/2, z-1/2; Symmetry code for **2**: #1 x-y+1, x, -z; #2 y, -x+y+1, -z; #3 -x+4/3, -x+y+2/3, -z+1/6; #4 -y+2, x-y+1, z; #5 -x+y+1, -x+2, z; #6 -x+2, -y+2, -z; #7 -x+y+1, -x+1, z; #8 -y+1, x-y, z; #9 -x+5/3, -y+4/3, -z+1/3.