Electronic Supplementary Material (ESI) for RSC Advances.

Spontaneous Chiral Resolution and Hierarchically Directing Effects of Two-winged Propeller-like SDAs on the Construction of Noncentrosymmetric Iodoargentates/Iodocuprates

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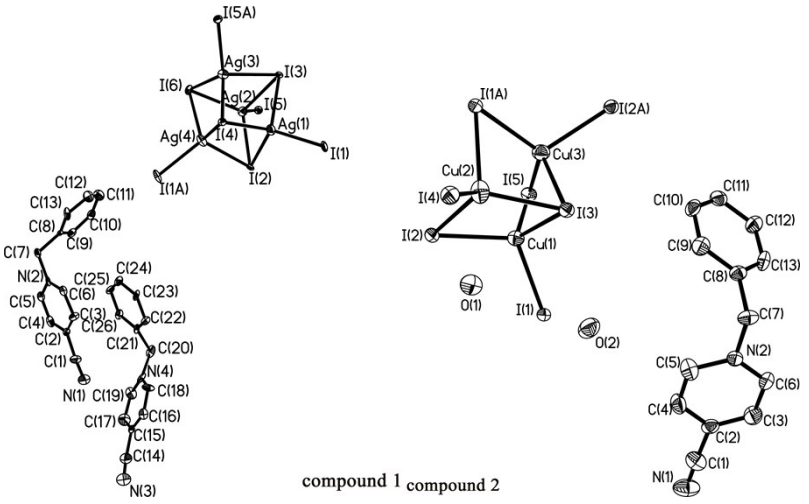
Supporting Information (SI)

Supporting Information of four compounds: Asymmetric unit diagram (Fig. S1)**,** EPR spectrum (Fig. S2), TG analyses (Fig. S3), Solid state optical diffuse–reflection spectra (Fig. S4), X–ray powder diffraction (XRPD) patterns (Fig. S5), Infrared Spectroscopy (Fig. S6), and selected bond lengths (Å) and angles (°) for **1**–**4** (Tables S1).



compound 1 compound 2

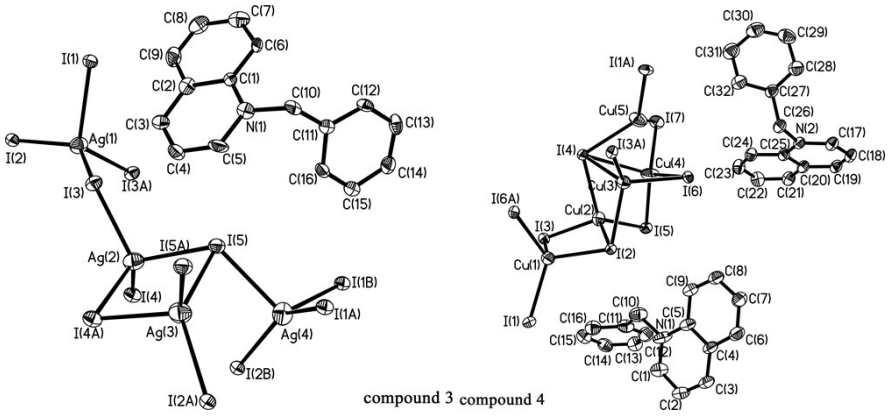


Fig. S1 Asymmetric unit diagram of **1**–**4** (H atoms are omitted for clarity).

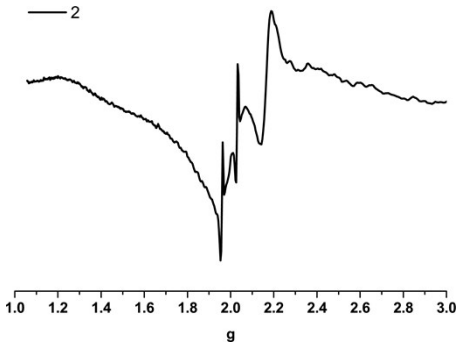


Fig. S2 EPR spectrum of 2 upon irradiation in the solid state.

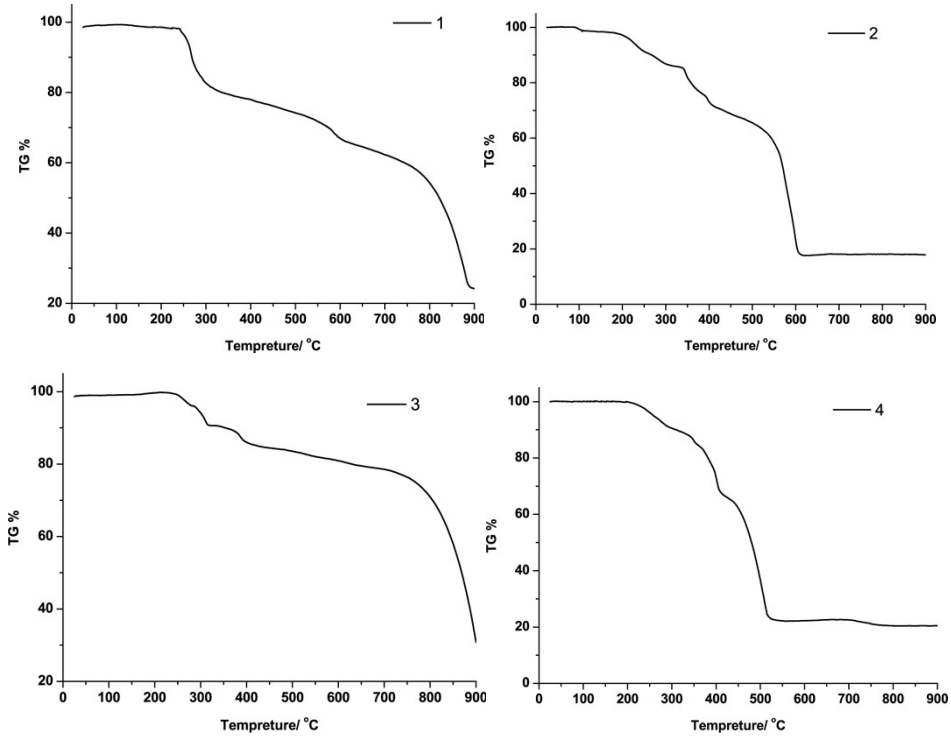


Fig. S3 TG curves for compounds **1**–**4**.

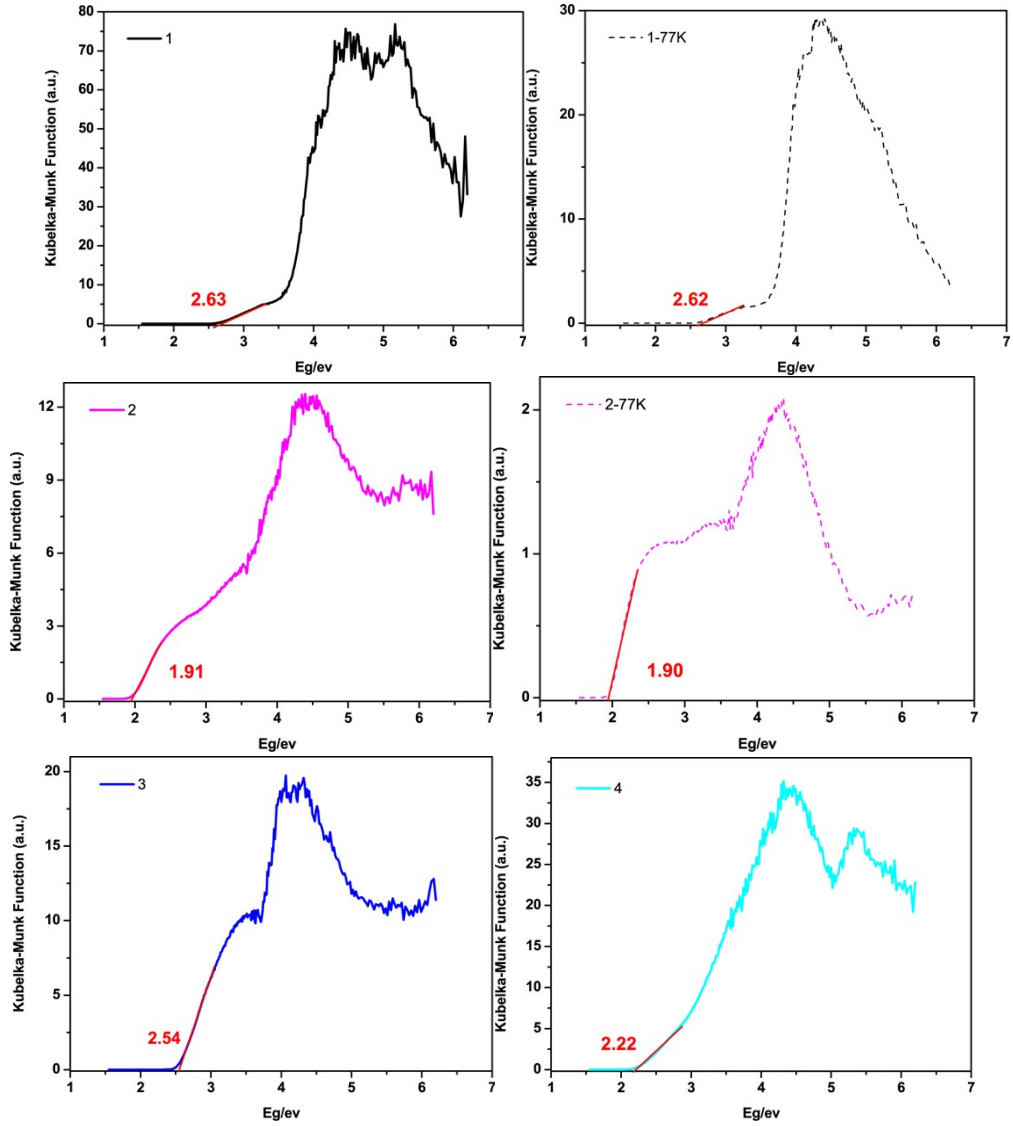
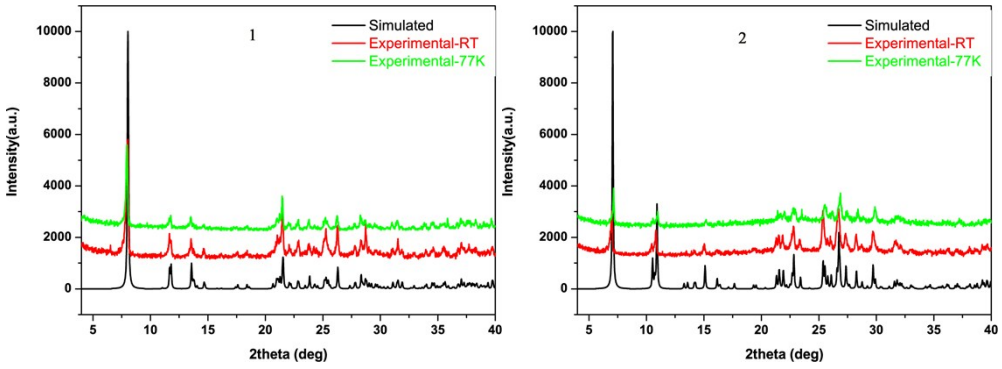


Fig. S4 Solid state optical diffuse-reflection spectra of **1**–**4** at room temperature and **1**–**2** at 77K.



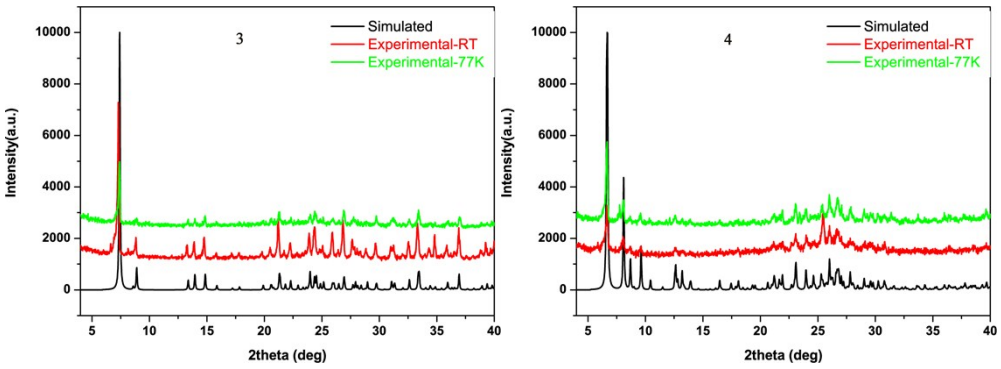


Fig. S5 X-ray powder diffraction (XRPD) patterns of **1**–**4** at room temperature (RT) and 77K.

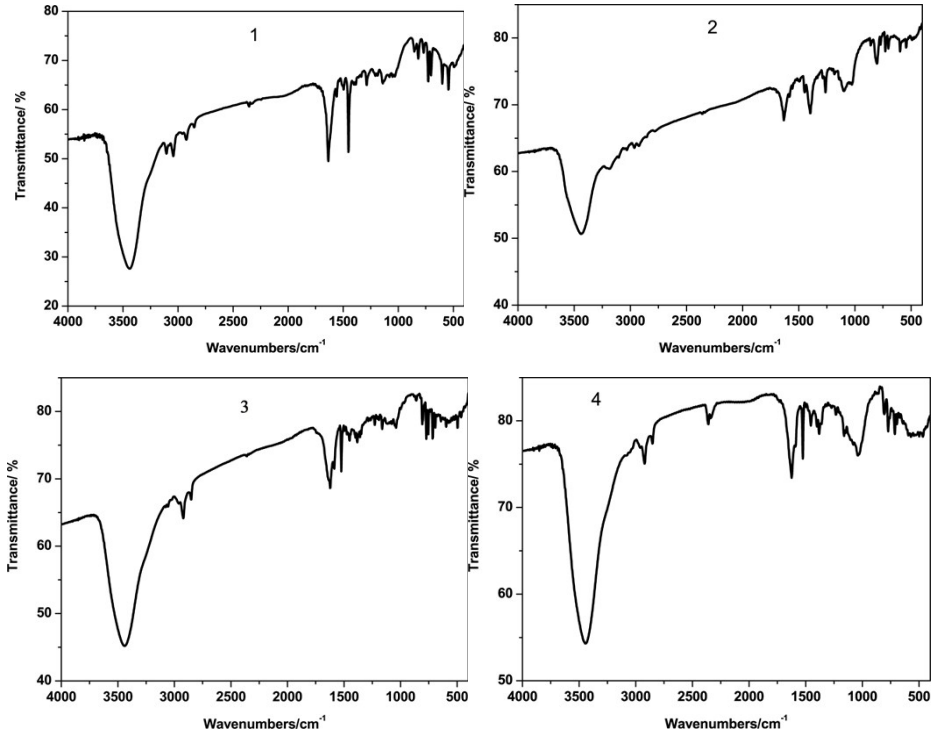


Fig. S6 IR spectra of **1**–**4**

Table S1. Selected bond lengths (Å) and angles (°) for **1**–**4** at 293(2) K

Compound 1			
Ag–I bond distances			
Ag(1)–I(1)	2.7913(9)	Ag(2)–I(5)	2.8326(9)
Ag(1)–I(2)	2.8845(12)	Ag(2)–I(2)	2.8576(10)
Ag(1)–I(4)	2.9041(7)	Ag(2)–I(6)	2.8806(7)
Ag(1)–I(3)	2.9153(10)	Ag(2)–I(3)	2.9325(10)
Ag(3)–I(5)#1	2.7967(12)	Ag(4)–I(1)#2	2.7551(10)
Ag(3)–I(6)	2.8525(10)	Ag(4)–I(4)	2.8548(12)
Ag(3)–I(4)	2.8949(10)	Ag(4)–I(6)	2.9566(12)
Ag(3)–I(3)	2.9082(6)	Ag(4)–I(2)	2.9654(10)
Ag…Ag distances			
Ag(1)–Ag(2)	3.2574(11)	Ag(2)–Ag(4)	3.1828(10)
Ag(1)–Ag(3)	3.4380(12)	Ag(3)–Ag(4)	3.3398(14)

Selected angles			
I(1)–Ag(1)–I(2)	113.58(4)	I(5)–Ag(2)–I(2)	105.38(3)
I(1)–Ag(1)–I(4)	117.60(3)	I(5)–Ag(2)–I(6)	116.34(3)
I(2)–Ag(1)–I(4)	104.83(2)	I(2)–Ag(2)–I(6)	114.20(2)
I(1)–Ag(1)–I(3)	106.95(3)	I(5)–Ag(2)–I(3)	109.44(2)
I(2)–Ag(1)–I(3)	108.49(3)	I(2)–Ag(2)–I(3)	108.75(3)
I(4)–Ag(1)–I(3)	104.80(3)	I(6)–Ag(2)–I(3)	102.55(3)
I(5)#1–Ag(3)–I(6)	121.62(3)	I(1)#2–Ag(4)–I(4)	122.69(3)
I(5)#1–Ag(3)–I(4)	111.30(3)	I(1)#2–Ag(4)–I(6)	106.97(3)
I(6)–Ag(3)–I(4)	108.01(3)	I(4)–Ag(4)–I(6)	106.28(4)
I(5)#1–Ag(3)–I(3)	105.37(3)	I(1)#2–Ag(4)–I(2)	107.47(4)
I(6)–Ag(3)–I(3)	103.86(3)	I(4)–Ag(4)–I(2)	104.01(3)
I(4)–Ag(3)–I(3)	105.22(3)	I(6)–Ag(4)–I(2)	108.89(3)
Symmetry code: #1 x,–y+2,z–1/2; #2 x–1/2,–y+5/2,z–1/2; #3 x+1/2,–y+5/2,z+1/2; #4 x,–y+2,z+1/2			

Compound 2			
Cu–I bond distances			
Cu(1)–I(5)	2.6470(16)	Cu(2)–I(4)	2.5842(17)
Cu(1)–I(2)	2.6763(17)	Cu(2)–I(2)	2.6662(18)
Cu(1)–I(3)	2.6840(15)	Cu(2)–I(3)	2.6838(19)
Cu(1)–I(1)	2.6912(17)	Cu(2)–I(1)#2	2.822(2)
Cu(3)–I(5)	2.6137(15)	Cu(3)–I(2)#2	2.6996(18)
Cu(3)–I(1)#2	2.6778(17)	Cu(3)–I(3)	2.7657(18)
Cu…Cu distances			
Cu(1)–Cu(2)	2.715(2)	Cu(1)–Cu(3)	2.856(2)
Cu(1)–Cu(3)#1	2.815(2)	Cu(2)–Cu(3)	3.014(2)
Cu(3)–Cu(1)#2	2.815(2)		
Selected angles			
I(5)–Cu(1)–I(2)	104.49(5)	I(4)–Cu(2)–I(2)	113.34(7)
I(5)–Cu(1)–I(3)	109.36(6)	I(4)–Cu(2)–I(3)	107.14(6)
I(2)–Cu(1)–I(3)	117.57(5)	I(2)–Cu(2)–I(3)	117.93(6)
I(5)–Cu(1)–I(1)	108.00(5)	I(4)–Cu(2)–I(1)#2	110.04(7)
I(2)–Cu(1)–I(1)	113.01(6)	I(2)–Cu(2)–I(1)#2	103.80(6)
I(3)–Cu(1)–I(1)	104.15(5)	I(3)–Cu(2)–I(1)#2	104.00(7)
I(5)–Cu(3)–I(1)#2	118.91(6)	I(5)–Cu(3)–I(3)	107.89(6)
I(5)–Cu(3)–I(2)#2	108.91(6)	I(1)#2–Cu(3)–I(3)	105.71(5)
I(1)#2–Cu(3)–I(2)#2	112.69(6)	I(2)#2–Cu(3)–I(3)	101.04(5)
Symmetry code: #1 -x+1,y-1/2,-z+1; #2 -x+1,y+1/2,-z+1			

Compound 3			
Ag–I bond distances			
Ag(1)–I(3)	2.7732(8)	Ag(2)–I(4)	2.7961(8)
Ag(1)–I(2)	2.8486(9)	Ag(2)–I(4)#3	2.8236(8)
Ag(1)–I(3)#1	2.8584(8)	Ag(2)–I(3)	2.8323(9)
Ag(1)–I(1)	2.9126(8)	Ag(2)–I(5)	2.9302(10)
Ag(3)–I(2)#4	2.8158(9)	Ag(4)–I(1)#4	2.7962(8)
Ag(3)–I(5)	2.8385(9)	Ag(4)–I(2)#5	2.9043(10)
Ag(3)–I(4)#3	2.8644(11)	Ag(4)–I(1)#5	2.9306(8)
Ag(3)–I(5)#3	3.1036(9)	Ag(4)–I(5)	2.9623(9)
Ag…Ag distances			
Ag(1)–Ag(4)#2	3.1614(9)	Ag(3)–Ag(2)#3	3.1522(11)
Ag(2)–Ag(3)#1	3.1522(11)	Ag(4)–Ag(1)#5	3.1614(9)
Selected angles			
I(3)–Ag(1)–I(2)	132.52(3)	I(4)–Ag(2)–I(4)#3	108.88(3)
I(3)–Ag(1)–I(3)#1	108.53(3)	I(4)–Ag(2)–I(3)	109.19(3)
I(2)–Ag(1)–I(3)#1	100.36(3)	I(4)#3–Ag(2)–I(3)	112.00(3)
I(3)–Ag(1)–I(1)	102.20(3)	I(4)–Ag(2)–I(5)	118.36(3)
I(2)–Ag(1)–I(1)	99.89(2)	I(4)#3–Ag(2)–I(5)	102.71(3)
I(3)#1–Ag(1)–I(1)	113.12(3)	I(3)–Ag(2)–I(5)	105.61(3)
I(2)#4–Ag(3)–I(5)	135.00(3)	I(1)#4–Ag(4)–I(2)#5	144.47(3)
I(2)#4–Ag(3)–I(4)#3	107.31(3)	I(1)#4–Ag(4)–I(1)#5	105.91(3)
I(5)–Ag(3)–I(4)#3	104.01(3)	I(2)#5–Ag(4)–I(1)#5	98.18(2)
I(2)#4–Ag(3)–I(5)#3	97.59(3)	I(1)#4–Ag(4)–I(5)	98.46(2)
I(5)–Ag(3)–I(5)#3	100.50(3)	I(2)#5–Ag(4)–I(5)	98.89(3)
I(4)#3–Ag(3)–I(5)#3	110.93(3)	I(1)#5–Ag(4)–I(5)	107.17(3)
Symmetry code: #1 x,y+1,z; #2 x–1/2,–y+2,z–1/2; #3 x,y–1,z; #4 x+1/2,–y+1,z+1/2; #5 x+1/2,–y+2,z+1/2; #6 x–1/2,–y+1,z–1/2			

Compound 4			
Cu–I bond distances			
Cu(1)–I(1)	2.6126(9)	Cu(2)–I(5)	2.6336(10)
Cu(1)–I(2)	2.6566(8)	Cu(2)–I(3)	2.6686(9)
Cu(1)–I(6)#1	2.7079(10)	Cu(2)–I(2)	2.6927(10)
Cu(1)–I(3)	2.7131(10)	Cu(2)–I(4)	2.7393(10)
Cu(3)–I(2)	2.6574(9)	Cu(4)–I(5)	2.5272(9)
Cu(3)–I(3)#2	2.6644(10)	Cu(4)–I(7)	2.5942(10)
Cu(3)–I(6)	2.6797(9)	Cu(4)–I(6)	2.6320(10)
Cu(3)–I(4)	2.6837(9)	Cu(4)–I(4)	3.0797(12)
Cu(5)–I(1)#2	2.5071(10)	Cu(5)–I(4)	2.6593(10)
Cu(5)–I(7)	2.6118(12)		
Cu…Cu distances			

Cu(1)–Cu(3)#1	2.8210(11)	Cu(2)–Cu(3)	2.9396(12)
Cu(1)–Cu(5)#1	2.9109(14)	Cu(3)–Cu(1)#2	2.8210(11)
Cu(1)–Cu(2)	2.9388(13)	Cu(4)–Cu(5)	2.5498(13)
Cu(2)–Cu(4)	2.8816(13)	Cu(5)–Cu(1)#2	2.9109(14)
Selected angles			
I(1)–Cu(1)–I(2)	111.66(3)	I(5)–Cu(2)–I(3)	110.13(3)
I(1)–Cu(1)–I(6)#1	118.27(4)	I(5)–Cu(2)–I(2)	110.80(3)
I(2)–Cu(1)–I(6)#1	97.18(3)	I(3)–Cu(2)–I(2)	112.47(3)
I(1)–Cu(1)–I(3)	107.55(3)	I(5)–Cu(2)–I(4)	117.07(4)
I(2)–Cu(1)–I(3)	112.20(3)	I(3)–Cu(2)–I(4)	100.39(3)
I(6)#1–Cu(1)–I(3)	109.82(3)	I(2)–Cu(2)–I(4)	105.62(3)
I(2)–Cu(3)–I(3)#2	110.48(4)	I(5)–Cu(4)–I(7)	125.43(4)
I(2)–Cu(3)–I(6)	105.26(3)	I(5)–Cu(4)–I(6)	109.19(3)
I(3)#2–Cu(3)–I(6)	112.20(3)	I(7)–Cu(4)–I(6)	112.97(3)
I(2)–Cu(3)–I(4)	108.23(3)	I(5)–Cu(4)–I(4)	109.25(4)
I(3)#2–Cu(3)–I(4)	108.85(3)	I(7)–Cu(4)–I(4)	94.52(3)
I(6)–Cu(3)–I(4)	111.72(4)	I(6)–Cu(4)–I(4)	101.72(4)
I(1)#2–Cu(5)–I(7)	125.93(4)	I(7)–Cu(5)–I(4)	104.94(3)
I(1)#2–Cu(5)–I(4)	120.15(4)		

Symmetry code: #1 –x+1/2,y+1/2,–z+1/2 #2 –x+1/2,y–1/2,–z+1/2