

Cuprous iodide coordination polymers (CuI)_x(L)_x·y(solvent) built on linear thioether linkers

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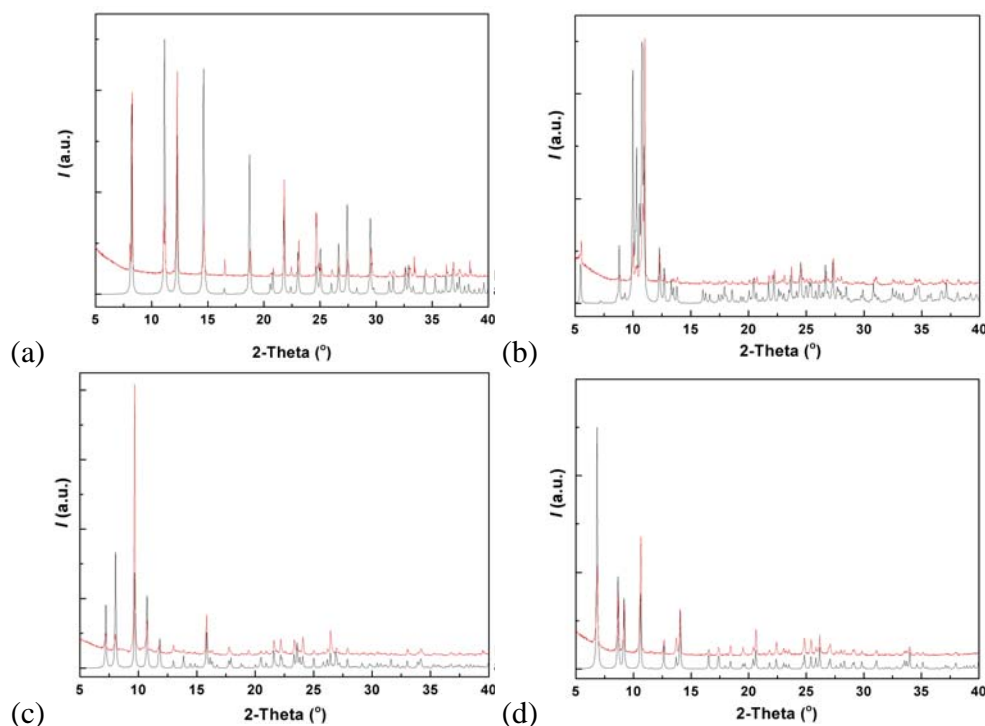


Fig. S1. Calculated (black) and experimental (red) PXRD patterns of MSF-6 (a), -7 (b), -8 (c) and -9 (d).

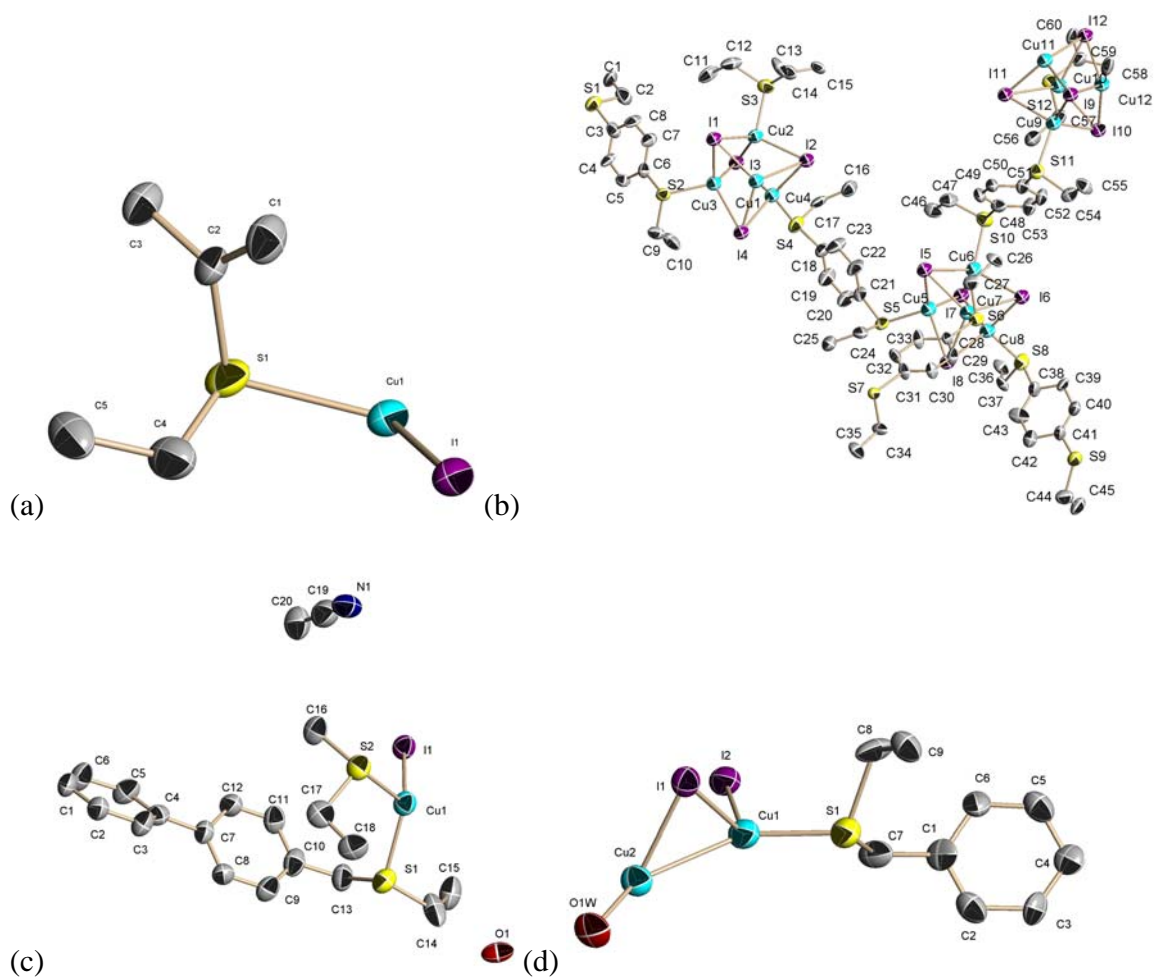


Fig. S2. ORTEP drawings of the asymmetric unit of (a) MSF-6, (b) MSF-7, (c) MSF-8 and (d) MSF-9, respectively, at the 50% probability. The H atoms are omitted for clarity.

Table S1. Some relevant interatomic lengths (Å) and angles (deg) for MSF-7

MSF-7							
Cu5—S5	2.317(3)	Cu6—I5	2.7420(14)	Cu9—S11	2.342(3)	Cu10—Cu11	2.7592(16)
Cu5—I5	2.6293(13)	Cu6—Cu8	2.8684(17)	Cu9—I11	2.6713(13)	Cu10—Cu12	2.8802(17)
Cu5—I7	2.6437(13)	Cu7—S6	2.328(3)	Cu9—I10	2.6779(14)	Cu11—S1 ⁱ	2.308(3)
Cu5—Cu6	2.6891(17)	Cu7—I8	2.6717(13)	Cu9—I9	2.6965(13)	Cu11—I11	2.6422(13)
Cu5—I8	2.7542(13)	Cu7—I6	2.6910(14)	Cu9—Cu10	2.7277(16)	Cu11—I12	2.6452(14)
Cu5—Cu8	2.8074(17)	Cu7—I5	2.7170(13)	Cu9—Cu12	2.7775(17)	Cu11—I9	2.7363(13)
Cu5—Cu7	2.8140(16)	Cu7—Cu8	2.7795(17)	Cu9—Cu11	2.8583(17)	Cu11—Cu12	2.7697(17)
Cu6—S10	2.317(3)	Cu8—S8	2.342(3)	Cu10—S12	2.318(3)	Cu12—S9 ^{iv}	2.318(3)
Cu6—I6	2.6473(13)	Cu8—I6	2.6552(14)	Cu10—I10	2.6727(13)	Cu12—I12	2.6638(13)
Cu6—I7	2.7274(13)	Cu8—I8	2.6625(14)	Cu10—I12	2.6991(13)	Cu12—I9	2.6703(13)
Cu6—Cu7	2.7360(16)	Cu8—I7	2.6890(13)	Cu10—I11	2.7093(14)	Cu12—I10	2.7189(13)
S7 ⁱⁱⁱ —Cu1—I4	109.50(7)	I3—Cu3—I4	114.89(5)	I5—Cu5—Cu6	62.06(4)	I10—Cu10—I11	114.10(5)
S7 ⁱⁱⁱ —Cu1—I1	107.91(7)	S2—Cu3—I1	99.72(7)	I7—Cu5—Cu6	61.51(4)	I12—Cu10—I11	111.31(4)
I4—Cu1—I1	114.71(5)	I3—Cu3—I1	109.44(4)	S5—Cu5—I8	99.28(7)	S1 ⁱ —Cu11—I11	113.31(8)
S7 ⁱⁱⁱ —Cu1—I2	107.95(7)	I4—Cu3—I1	110.84(4)	I8—Cu8—I7	111.96(5)	S1 ⁱ —Cu11—I12	105.70(9)
I4—Cu1—I2	108.45(4)	S4—Cu4—I2	116.69(8)	S11—Cu9—I11	104.93(7)	I11—Cu11—I12	115.25(5)
I1—Cu1—I2	108.14(4)	S4—Cu4—I4	106.29(9)	S11—Cu9—I10	103.84(7)	S1 ⁱ —Cu11—I9	103.00(8)
S3—Cu2—I2	106.23(8)	I2—Cu4—I4	110.01(4)	I11—Cu9—I10	115.20(5)	I11—Cu11—I9	106.62(4)
S3—Cu2—I1	108.65(8)	S4—Cu4—I3	100.13(8)	S11—Cu9—I9	112.90(7)	I12—Cu11—I9	112.39(5)
I2—Cu2—I1	110.93(4)	I2—Cu4—I3	110.41(4)	I11—Cu9—I9	106.94(4)	S9 ^{iv} —Cu12—I12	104.24(8)
S3—Cu2—I3	108.92(8)	I4—Cu4—I3	113.05(5)	I10—Cu9—I9	112.89(5)	S9 ^{iv} —Cu12—I9	118.85(8)
I2—Cu2—I3	110.51(4)	S5—Cu5—I5	112.46(7)	S12—Cu10—I10	109.15(7)	I12—Cu12—I9	113.94(5)
I1—Cu2—I3	111.43(5)	S5—Cu5—I7	106.24(8)	S12—Cu10—I12	108.06(8)	S9 ^{iv} —Cu12—I10	98.79(8)
S2—Cu3—I3	115.56(7)	I5—Cu5—I7	118.39(5)	I10—Cu10—I12	107.31(5)	I12—Cu12—I10	106.99(4)
S2—Cu3—I4	105.33(7)	S5—Cu5—Cu6	152.69(8)	S12—Cu10—I11	106.76(8)	I9—Cu12—I10	112.41(5)

Symmetry transformations: (i) -x, -y, 1-z; (ii) -x, 1-y, 2-z; (iii) 2-x, -y, 1-z; (iv) 2-x, 1-y, 2-z.