

A New Three-Dimensional Two-Fold Interpenetrated Framework with sqp Net Based on Cu₆I₆ and Cu₈I₈ Cluster Nodes

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Table. S1. Selected bond lengths (Å) for the title compound.

Cu(1)-I(1)	2.801(3)	Cu(7)-I(8)	2.6034(16)
Cu(1)-I(2)	2.5983(13)	Cu(8)-I(7)	2.6544(15)
Cu(2)-I(1)	2.6133(12)	Cu(8)-I(8)	2.7162(16)
Cu(2)-I(2)	2.6791(12)	Cu(8)-I(9)	2.6937(10)
Cu(2)-I(3)	2.6435(14)	Cu(9)-I(8)	2.6863(12)
Cu(3)-I(2)	2.6884(13)	Cu(9)-I(9)	2.6379(11)
Cu(3)-I(3)	2.6497(13)	Cu(9)-I(10)	2.6513(11)
Cu(3)-I(4)	2.6253(12)	Cu(10)-I(9)	2.6917(10)
Cu(4)-I(3)	2.6892(12)	Cu(10)-I(10)	2.7812(17)
Cu(4)-I(4)	2.628(2)	Cu(2)-N(2)	2.099(5)
Cu(5)-I(5)	2.6925(19)	Cu(3)-N(3)	2.128(6)
Cu(5)-I(6)	2.7532(11)	Cu(4)-N(7)#1	2.146(10)
Cu(6)-I(5)	2.6428(12)	Cu(5)-N(5)	2.189(10)
Cu(6)-I(6)	2.6335(12)	Cu(6)-N(4)#2	2.107(6)
Cu(6)-I(7)	2.7513(13)	Cu(9)-N(1)	2.099(6)
Cu(7)-I(6)	2.7270(11)	Cu(10)-N(6)	2.089(9)
Cu(7)-I(7)	2.7475(18)		

Symmetry codes: #1 -x+3/2, -y+2, z-1/2; #2 x-1, y, z.

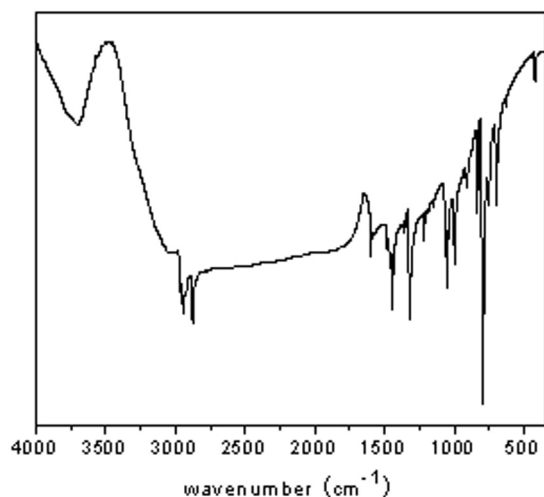


Fig. S1. The IR spectrum of the title compound.

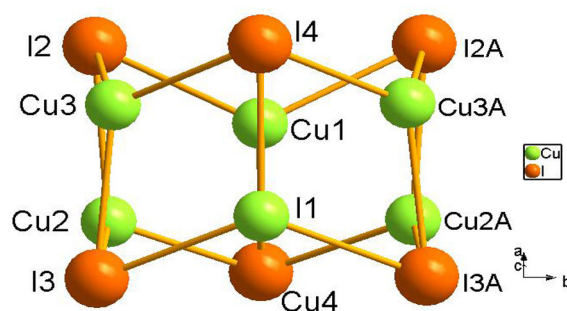


Fig. S2 The Cu₆I₆ cluster unit.

As shown in Fig. S2, Cu2A, Cu3A, I2A, I3A are obtained from Cu2, Cu3, I2, I3 by mirror symmetry. Cu1, I4, I1 and Cu4 just lie on the mirror plane perpendicular to the *b* axis. The neighboring Cu₆I₆ units are obtained by the translation along *a*, *b*, *c* direction, respectively.

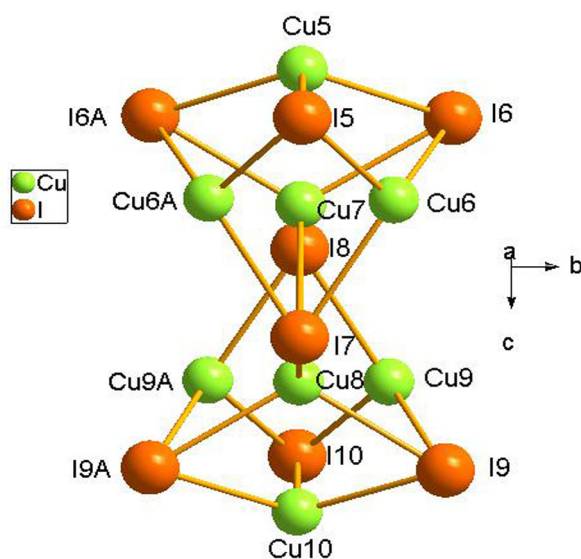


Fig. S3. The Cu₈I₈ cluster unit.

As shown in Fig. S3. Cu6A, I6A, Cu9A, I9A are obtained from Cu6, I6, Cu9, I9 by mirror symmetry. Cu5, I5, Cu7, I8, I7, Cu8, I10 and Cu10 just lie on the mirror plane perpendicular to the *b* axis. The neighboring Cu₈I₈ units are obtained by the translation along *a*, *b*, *c* direction, respectively.

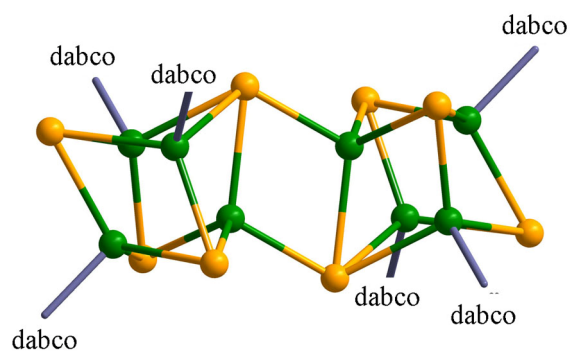


Fig. S4. The Cu₈I₈ cluster unit in the reported compound for comparison.

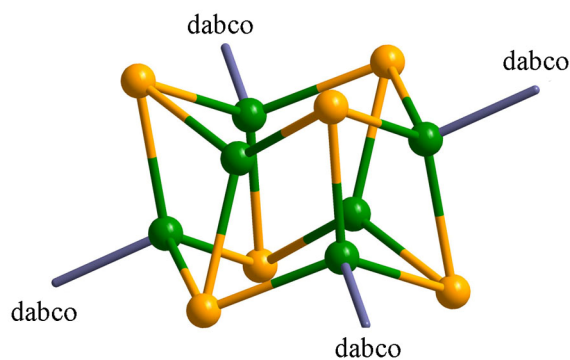


Fig. S5. The Cu₆I₆ cluster unit in the reported compound for comparison.

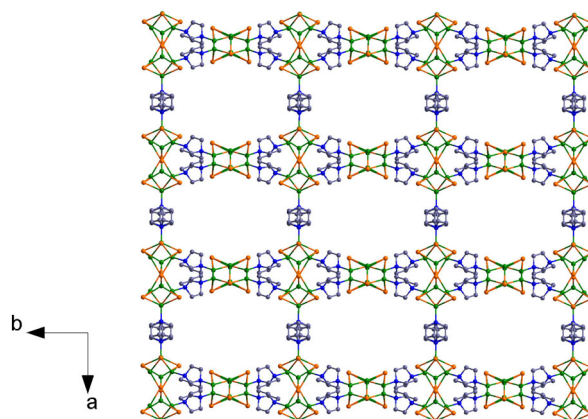


Fig. S6. The 3-D network of the reported compound in the *ab* plane, showing the arrangement and connecting between the layers, which is different from the situation in the title compound.

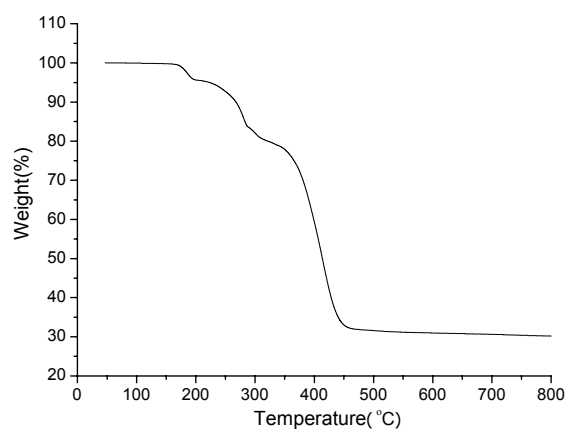


Fig. S7. TGA curve of the title compound