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Construction and characterization of an inorganic-organic hybrid copper(I) iodide coordination polymer with the semiconducting luminescence

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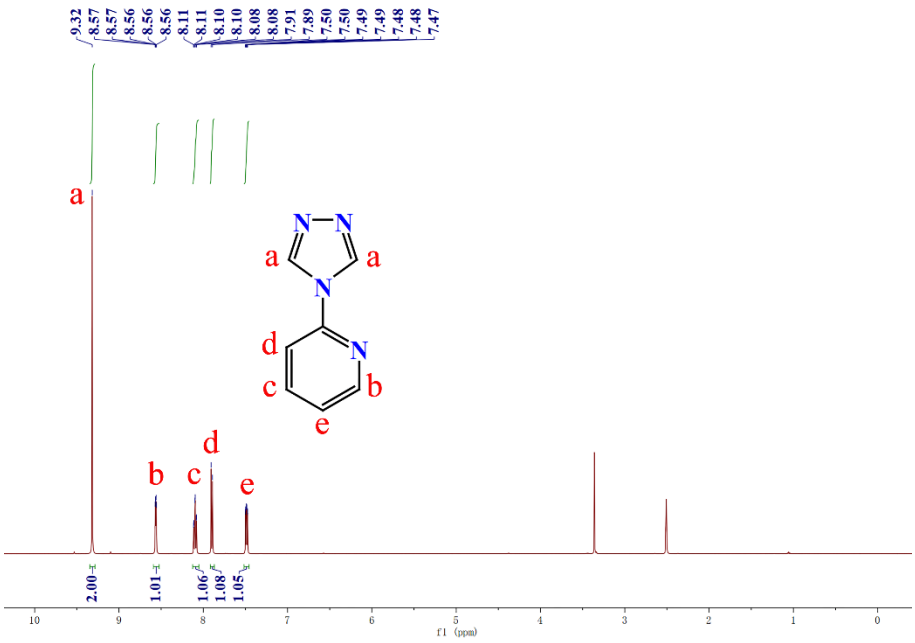

Fig. S1. The ^{1}H NMR spectrum of Pytz in DMSO-d_6.

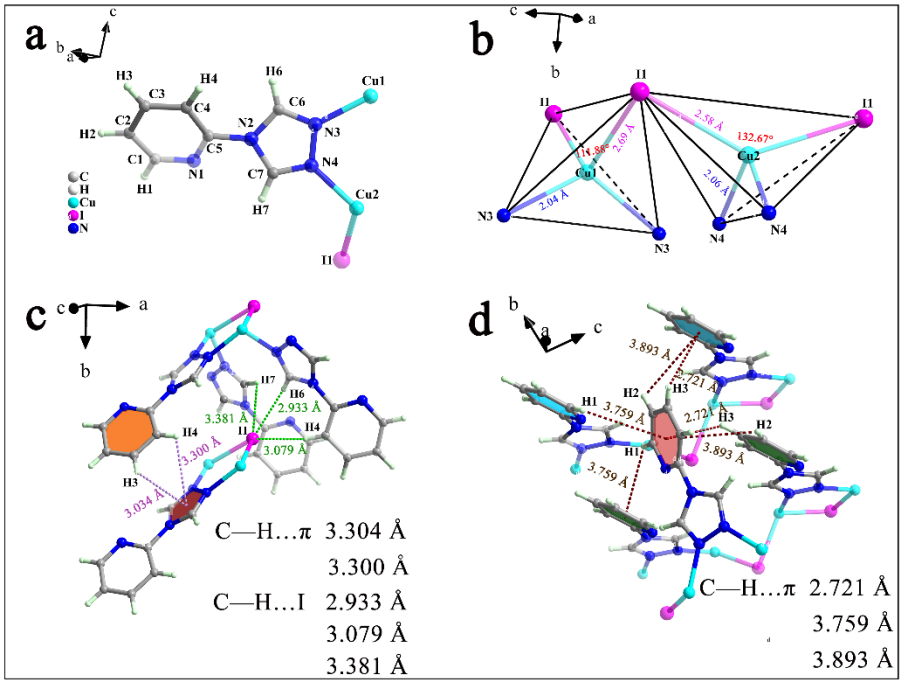

Fig. S2. (a) The asymmetric unit of CuI-Pytz. (b) The distorted tetrahedrons of CuI-Pytz. (c) and (d) The illustrtion of the C-H…π and C-H…I interactions stabilizing the supramolecular structure.

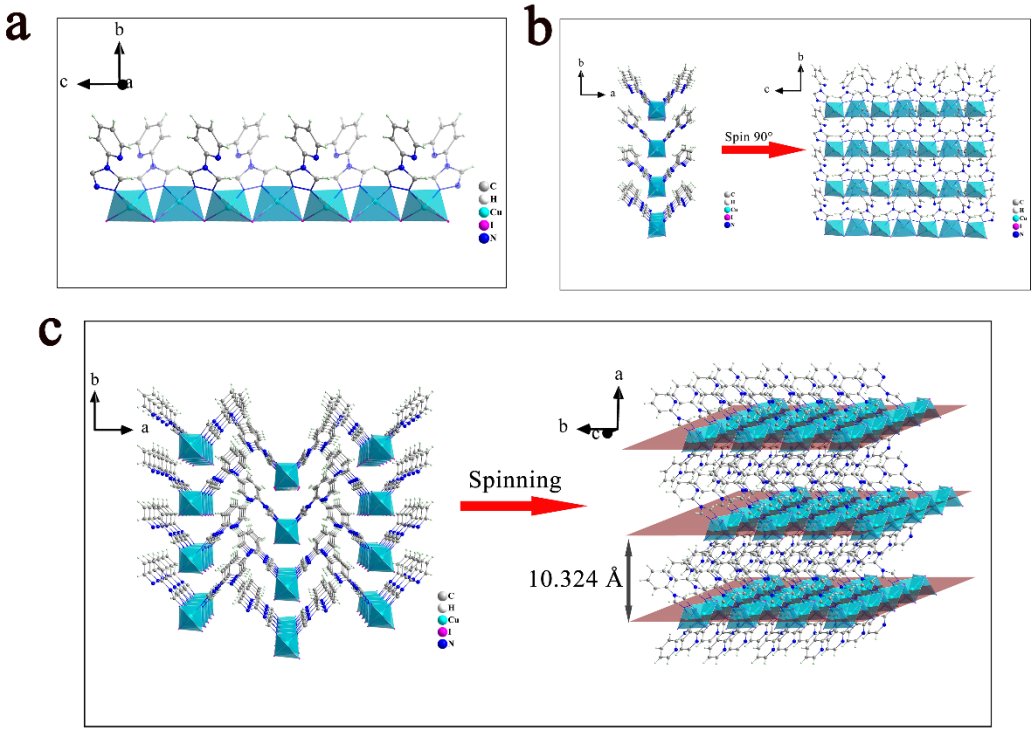

Fig. S3. (a) 1D chain of CuI-Pytz. (b) 2D layer of CuI-Pytz. (c) 3D structure of CuI-Pytz.

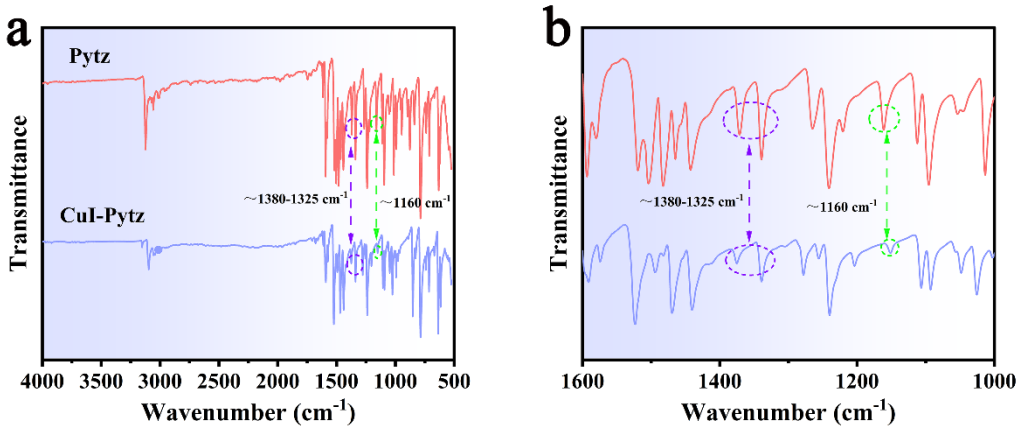

Fig. S4. (a) FT-IR spectra of Pytz and CuI-Pytz. (b) The fine structure of IR spectra.

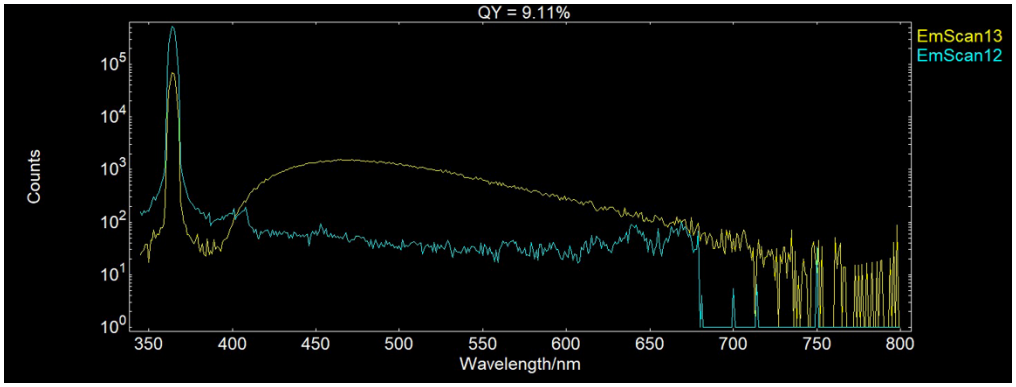

Fig. S5. The PL quantum yield (Φ_{PL}) of CuI-Pytz under 365 nm excitation light.

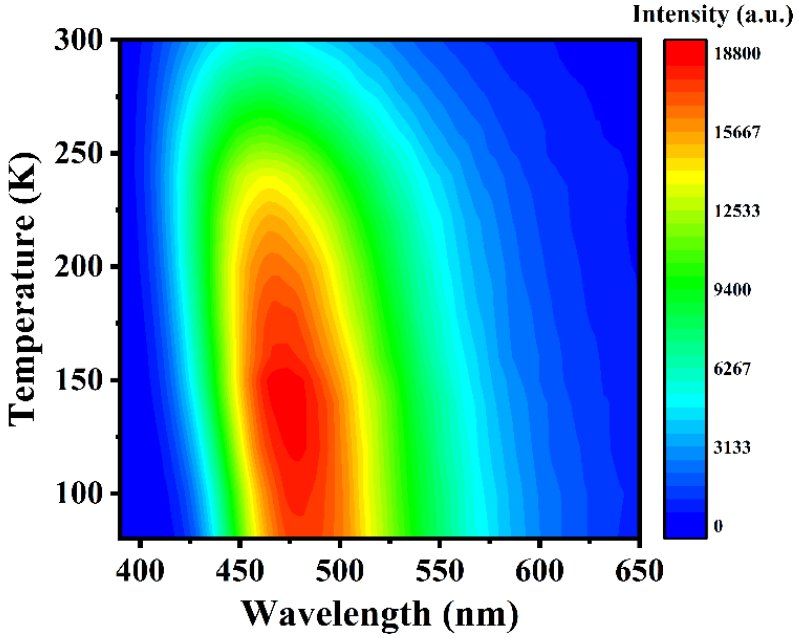

Fig. S6. Temperature and PL emission 2D contour mapping.

Table S1. Selected bond lengths (Å) and bond angles (°) for **CuI-Pytz**.

Cu1—I1[1]	2.6879(4)	N3[3]—Cu1—I1[1]	117.04(8)
Cu1—I1[2]	2.6879(4)	N3—Cu1—I1[1]	99.51(8)
Cu1—N3	2.042(3)	N3—Cu1—I1[2]	117.04(8)
Cu1—N3[3]	2.041(3)	N3[3]—Cu1—N3	112.81(16)
Cu2—I1	2.5809(3)	I1[1]—Cu2—I1	132.67(3)
Cu2—I1[2]	2.5809(3)	N4[1]—Cu2—I1	100.09(8)
Cu2—N4	2.059(3)	N4[1]—Cu2—I1[1]	109.72(8)
Cu2—N4[2]	2.059(3)	N4—Cu2—I1	109.72(8)
I1[1]—Cu1—I1[2]	111.88(2)	N4—Cu2—I1[1]	100.09(8)
N3[3]—Cu1—I1[2]	99.51(8)	N4—Cu2—N4[1]	100.66(16)

Symmetry codes: [1]+X, +Y, 1+Z; [2]1-X, +Y, 1-Z; [3]1-X, +Y, 2-Z (Bond lengths).

[1]1-X, +Y, 1-Z; [2]+X, +Y, 1+Z; [3]1-X, +Y, 2-Z; [4]+X, +Y, -1+Z (Bond angles).

Table S2. Temperature-dependent lifetime values of **CuI-Pytz**.

Temp (K)	**A_1**	**τ_1 (μs)**	**A_2**	**τ_2 (μs)**	**τ_{ave} (μs)**
80	0.684 (50%)	24.500	0.684 (50%)	29.945	27.495
100	0.699 (50%)	21.439	0.699 (50%)	26.203	24.059
120	0.741 (50%)	17.902	0.741 (50%)	21.880	20.089
140	0.864 (50%)	14.059	0.864 (50%)	17.183	15.777
160	0.982 (50%)	11.054	0.982 (50%)	13.510	12.405
180	0.800 (50%)	9.880	0.800 (50%)	12.075	11.087
200	0.290 (30.8%)	3.033	0.651 (69.2%)	7.382	6.709
220	0.340 (36.4%)	1.972	0.594 (63.6%)	5.587	4.980
240	0.386 (40.8%)	1.603	0.561 (59.2%)	4.431	3.868
260	0.403 (43.2%)	1.058	0.529 (56.8%)	3.219	2.786
280	0.367 (39.2%)	0.623	0.569 (60.8%)	2.141	1.901
300	0.379 (41.2%)	0.381	0.541 (58.8%)	1.310	1.153