Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting info

White luminescence achieved by a multiple thermochromic emission in a hybrid organic-inorganic compound based on 3-picolylamine and Copper(I) Iodide.

F. Farinella,[a] L. Maini,[a*] P.P. Mazzeo,[b*] V. Fattori,[c] F. Monti,[c*] and D. Braga[a]

[a.] *Dipartimento di Chimica "G. Ciamician", Università di Bologna, Via F. Selmi 2, Bologna, Italy.*
[b.] *Paul Scherrer Institut, Swiss Light Source, Villigen PSI 5232, Switzerland.*
[c.] *Istituto per la Sintesi Organica e la Fotoreattività (ISOF)-CNR, Via Gobetti 101, 40129, Bologna, Italy.*

TGA analysis of $[Cu_2I_2(3pica)]_\infty$

The TGA analysis of $[Cu_2I_2(3pica)]_\infty$ (Fig 1) reveals that the complex is stable up to 210°C which corresponds to decomposition temperature. No other crystalline phases have been detected. Both of the losses below 400°C were assigned to the release of the ligand.

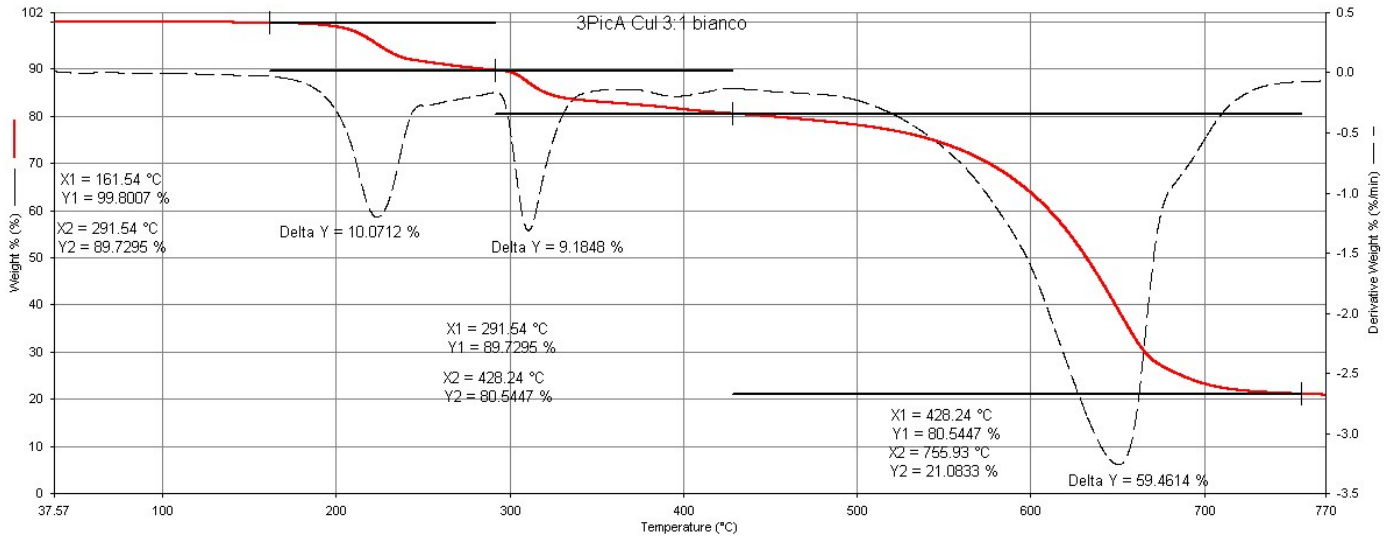
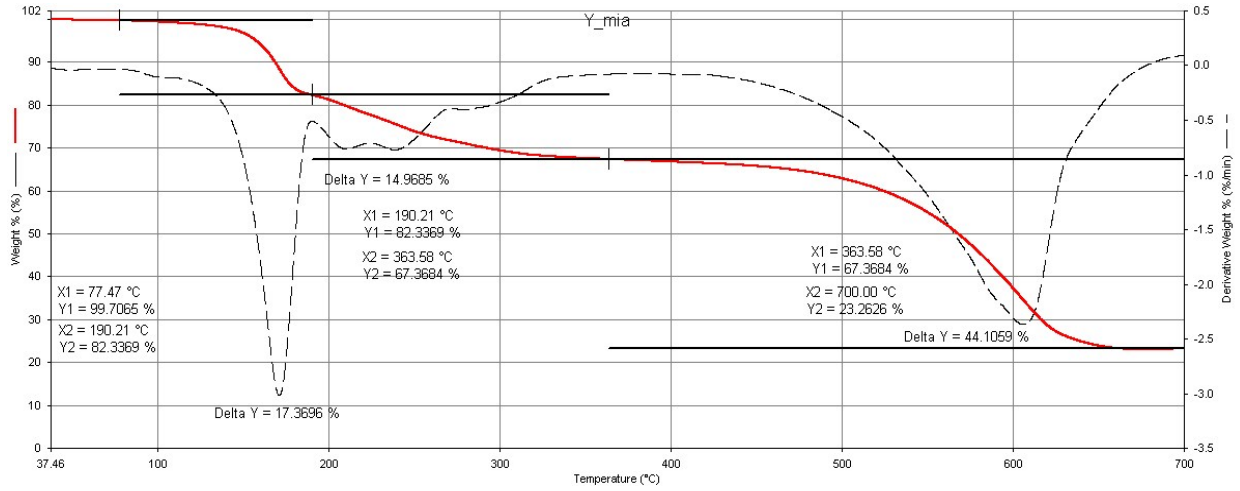


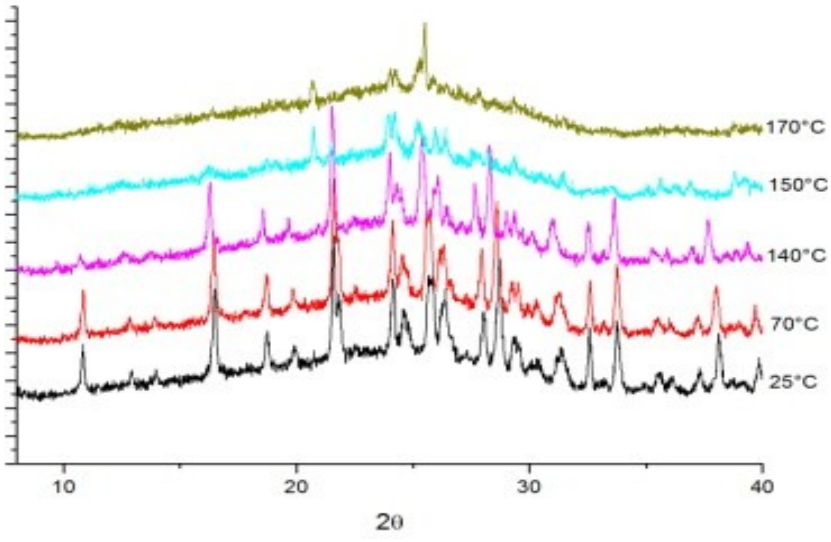
Fig. 1: TGA analysis of crystalline $Cu_2I_2(3pica)_\infty$

TGA analysis of [CuI(3pica)]

The TGA analysis of the complex [CuI(3pica)] (fig 2a) shows a first weight loss of 17.7% which corresponds to the release of one ligand. From the variable temperature XRPD (fig 2b) we have indications of the thermal stability of the complex, in fact a progressive decomposition of the powder is observed, up to the amorphization which occurred at 170 °C.



a

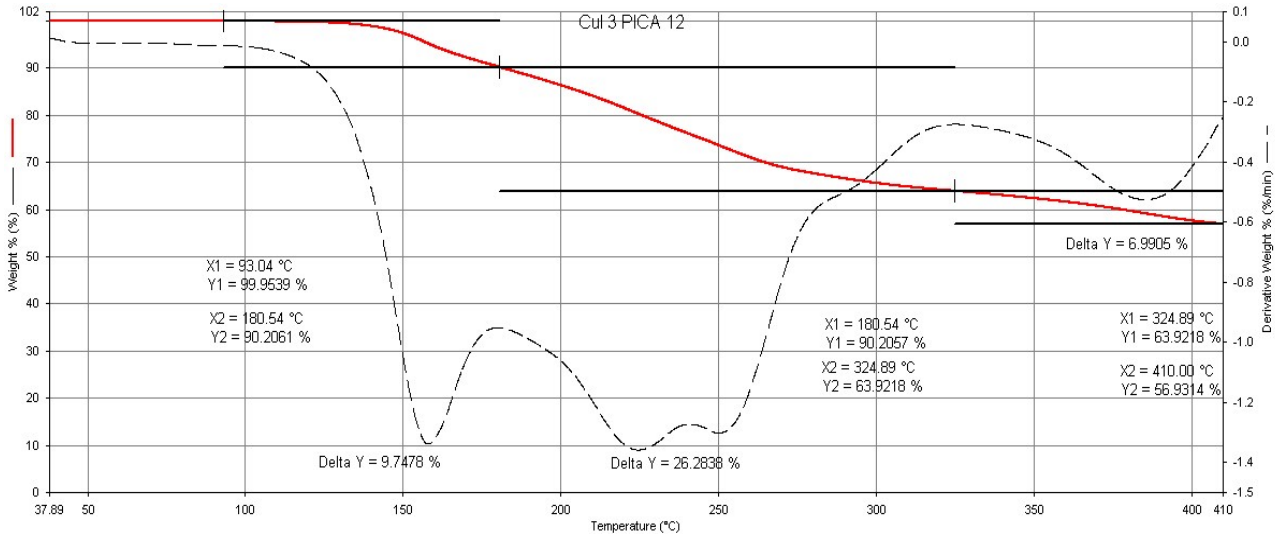


b

Fig. 2: a) TGA of crystalline [CuI(3pica)]; b) comparison of the powder pattern at different temperature for crystalline [CuI(3pica)].

TGA analysis of [CuI(3pica)](CH_3CN)

The TGA analysis of the complex [CuI(3pica)] (CH_3CN) (fig 3a) shows a total weight loss of 37%, below 300°C, which corresponds to the release of the solvent and the ligand. From the variable temperature XRPD (fig 3b) we have indications of the thermal stability of the complex, in fact a progressive decomposition of the powder is observed, up to the amorphization which occurred at 170 °C together with the loss of the solvent.



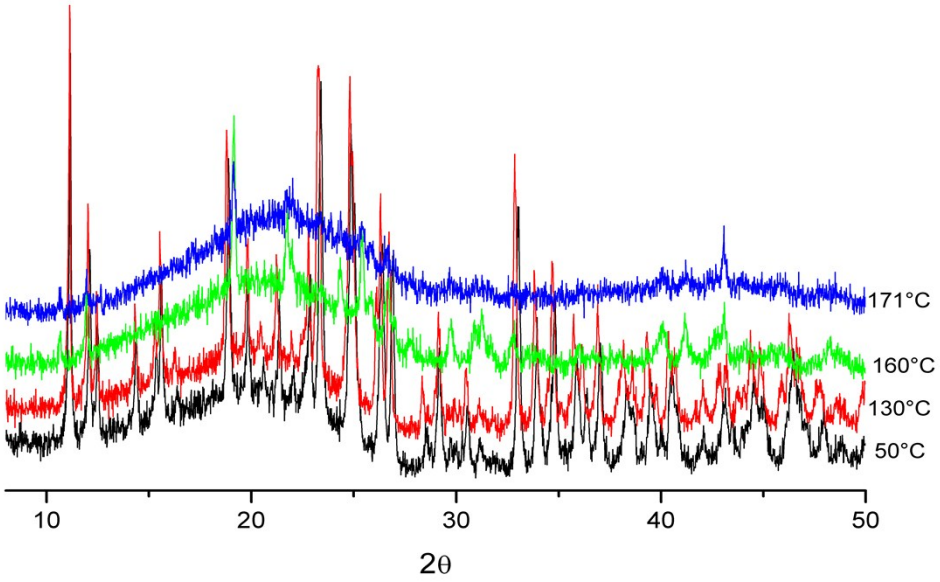


Fig. 3: a) TGA of crystalline [CuI(3pica)]; b) comparison of the powder pattern at different temperature for crystalline [CuI(3pica)] (CH_3CN).

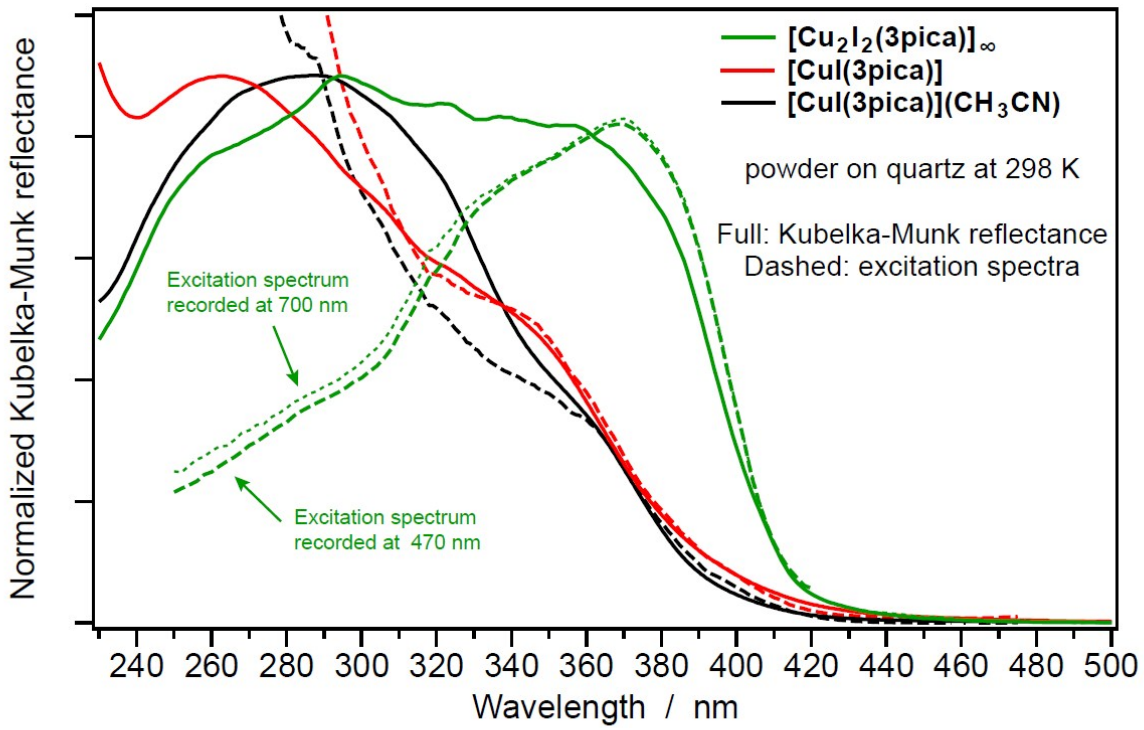


Fig. 4: Comparison between the diffuse reflectance spectra (elaborated using the Kubelka-Munk function) and the excitation spectra of all the investigated Cu(I) complexes in solid state, as neat powder on quartz slides. All the excitation spectra were recorded at emission maximum, except for the white-emitting complex [CuI(3pica)](CH_3CN). In that case, two different emission wavelengths were selected (*i.e.*, one on the ^{1,3}(X+MLCT) and the other on the ^{3}CC band) in order to rule out the presence of emitting impurities.

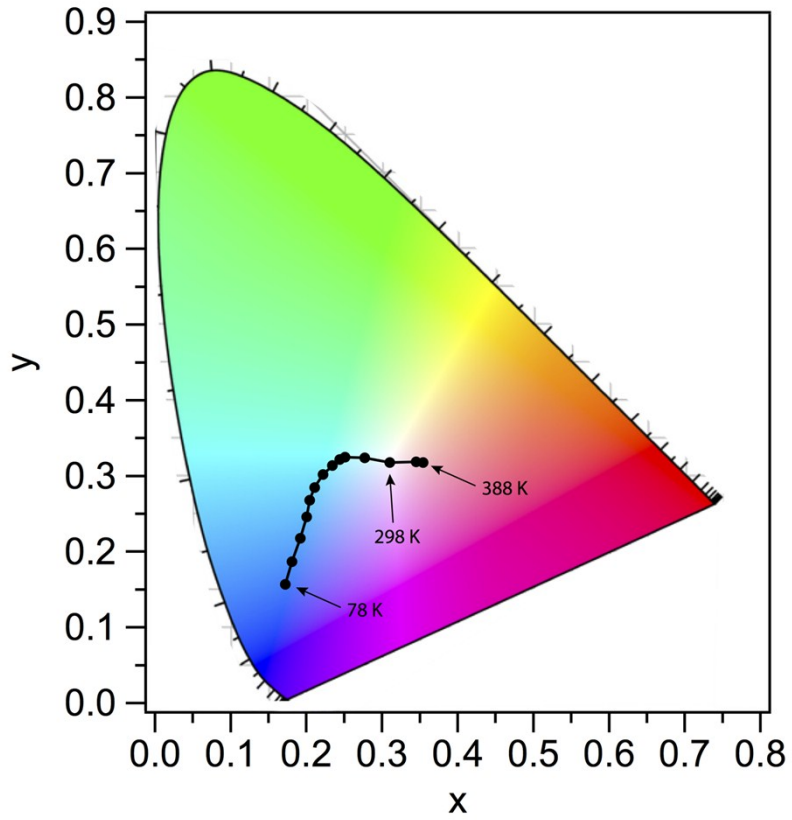


Fig. 5: Variation in the emission color of $[Cu_2I_2(3pica)]_\infty$ with temperature. The CIE coordinates on the chromaticity diagram are calculated from the corrected emission spectra reported in Figure 7 of the main text.