Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Synthesis of dual emitting iodocuprates: can solvent switch the reaction outcome?

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X-Ray crystallography data

Single crystals of **1** were grown by slow evaporation of an acetonitrile solution at room temperature for overnight. Crystals of **2** were obtained in a similar way using an acetone solution. The data were collected on a Bruker Kappa Apex II CCD diffractometer using ϕ,ω-scans of narrow (0.5°) frames with MoKα radiation (λ = 0.71073 Å) and a graphite monochromator. Experiments were carried out both at 296 K (structures **1** and **2**) and at a low temperature (structures **LT-1** and **LT-2**). The structures were solved by direct method and refined by a full matrix least-squares anisotropic-isotropic (for H atoms) procedure using *SHELXL-2014/7* program set.[1] Absorption corrections were applied using the empirical multiscan method with the *SADABS* program.[2] The positions of the hydrogen atoms were calculated with the riding model. The crystallographic data and details of the structure refinements are summarized in Table S1.

Table S1. Crystal data and structure refinement for **1**, **LT-1**, **2**, and **LT-2**.

	1	**LT-1**	**2**	**LT-2**
CCDC number	1980260	1980261	1980262	1980263
Chemical formula	$C_7H_{10}Cu_2I_3NS$	$C_7H_{10}Cu_2I_3NS$	$C_7H_{10}Cu_2I_3NS$	$C_7H_{10}Cu_2I_3NS$
M_r	648.00	648.00	552.78	552.78
Crystal system, space group	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Monoclinic, $C2/c$	Monoclinic, $C2/c$
Temperature (K)	296	150	296	173
a, b, c (Å)	8.3955(6), 8.8269(6), 10.2082(7)	8.3509(5), 8.6611(5), 10.1643(6)	17.1423(7), 12.6156(5), 14.4514(9)	17.0938(6), 12.5931(3), 14.2965(5)
α, β, γ (°)	83.171(3), 80.856(3), 78.317(3)	83.349(2), 81.897(2), 78.881(2)	90, 125.098(2), 90	90, 125.166(1), 90
V (Å^3)	728.46(9)	711.18(7)	2557.0(2)	2515.83(14)
Z	2	2	8	8
μ (mm^{-1})	9.39	9.62	8.68	8.82
Crystal size (mm)	0.50 × 0.30 × 0.10	0.35 × 0.22 × 0.06	0.35 × 0.10 × 0.02	0.15 × 0.15 × 0.10
T_{min}, T_{max}	0.578, 0.862	0.510, 0.928	0.618, 0.928	0.510, 0.928
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10792, 3290, 2575	12728, 3745, 3186	29378, 3740, 3223	15875, 4593, 3941
R_{int}	0.022	0.033	0.044	0.049
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.704	0.705	0.759
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.133, 1.01	0.031, 0.075, 1.03	0.033, 0.083, 1.03	0.030, 0.078, 1.03
No. of reflections	3290	3745	3740	4593
No. of parameters	139	139	121	121
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	2.31, –1.63	1.92, –1.53	1.96, –2.14	2.42, –2.93

[1] G. M. Sheldrick, *Acta Crystallogr., Sect. C: Struct. Chem.*, **2015**, *71*, 3–8.
[2] *SADABS*, v. 2008-1, Bruker AXS, Madison, WI, USA, 2008.

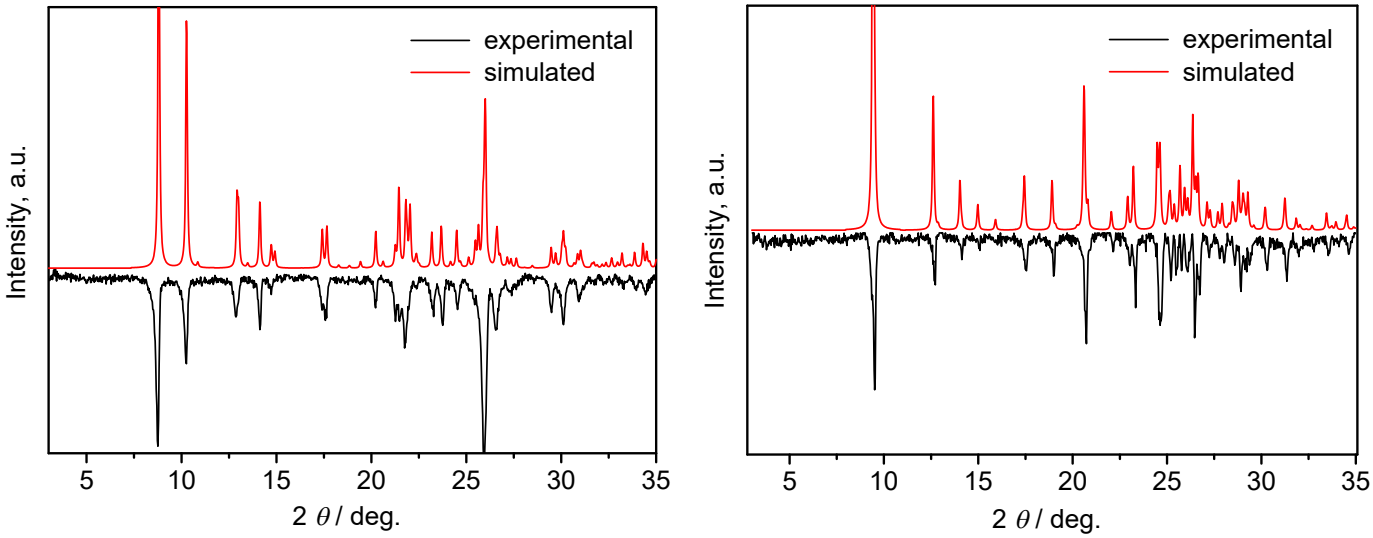


Figure S1. Experimental and simulated PXRD patterns of as-made samples of **1** (*left*) and **2**.

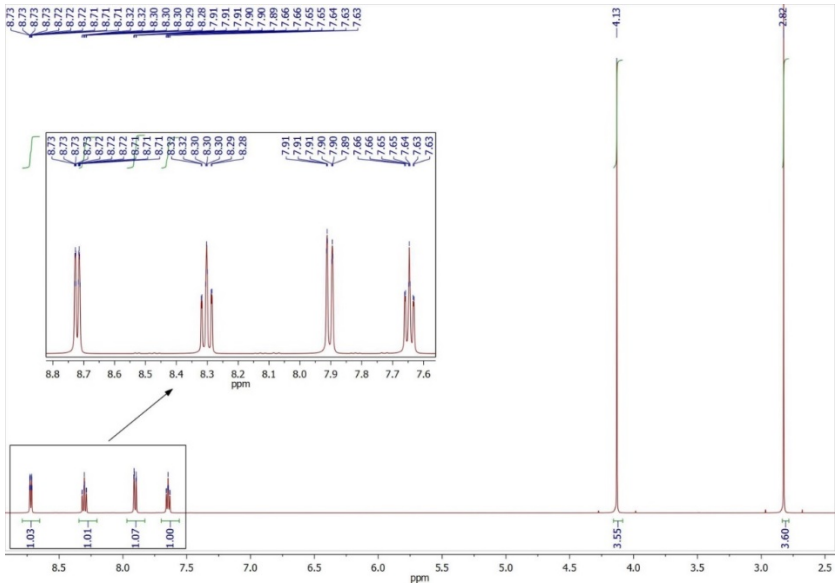


Figure S2. ^{1}H NMR spectrum of **[Me-PySMe]I** (CD_3CN).

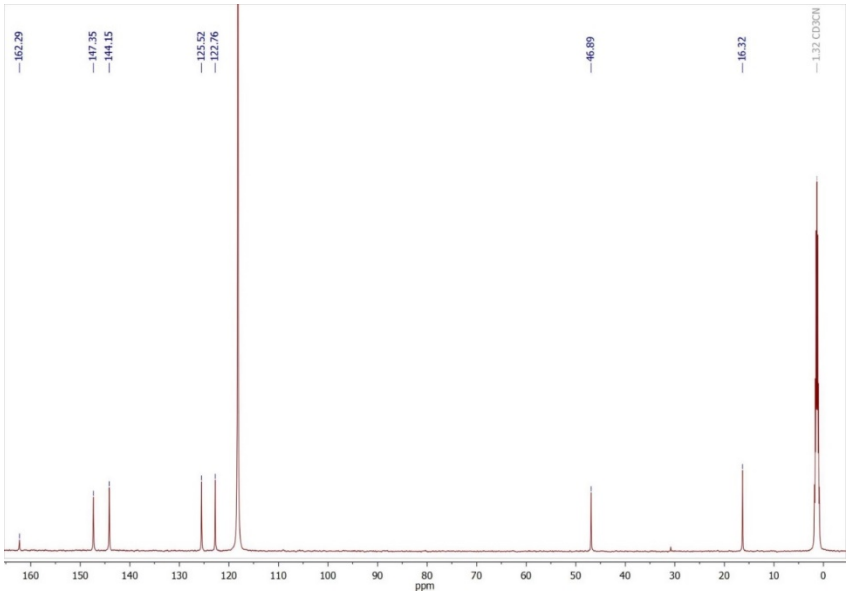


Figure S3. ^{13}C NMR spectrum of **[Me-PySMe]I** (CD_3CN).

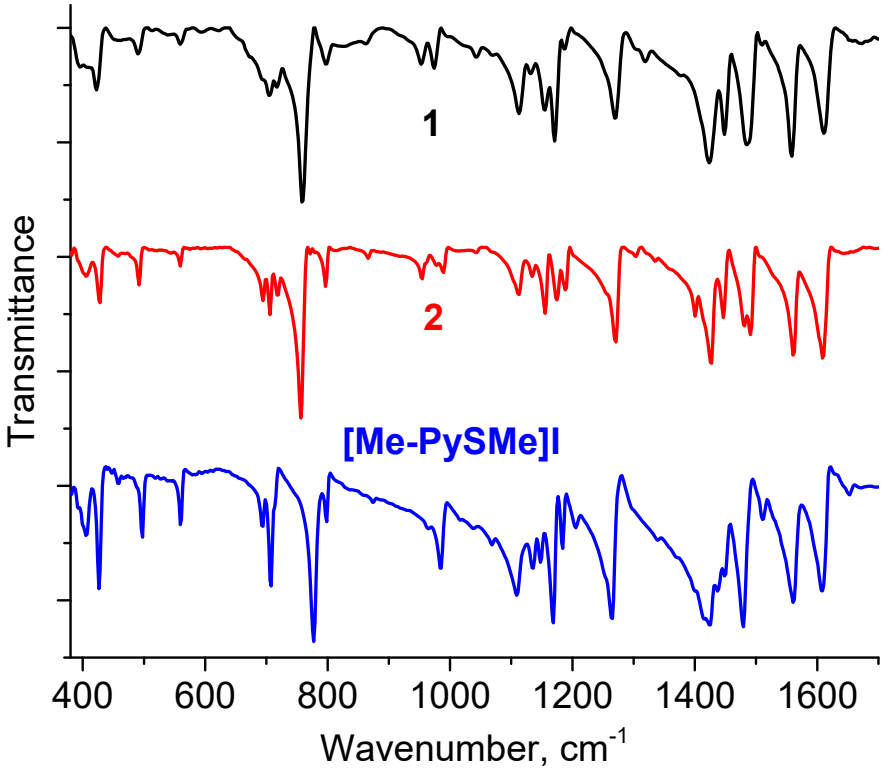


Figure S4. FT-IR spectra of **1**, **2** and **[Me-PySMe]I** showed in the fingerprint region.

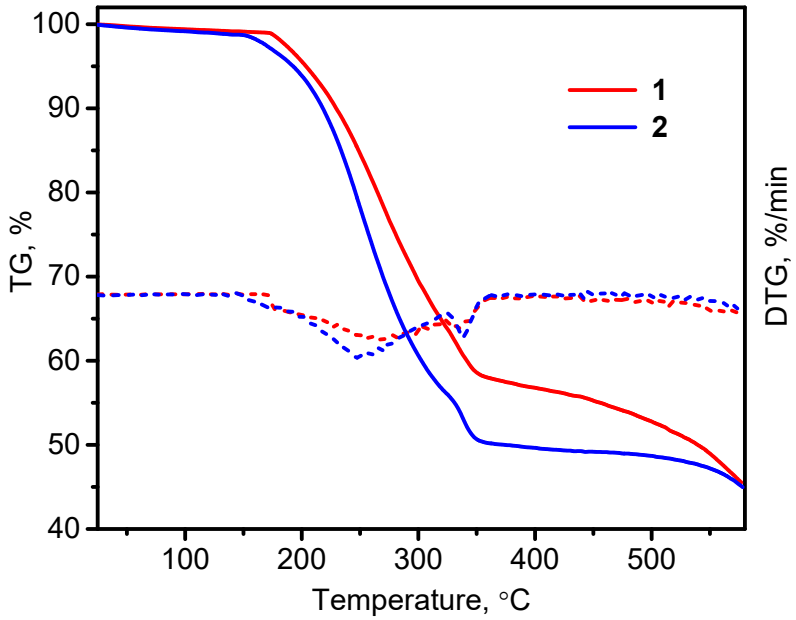


Figure S5. TGA&DTG curves for **1** and **2**.

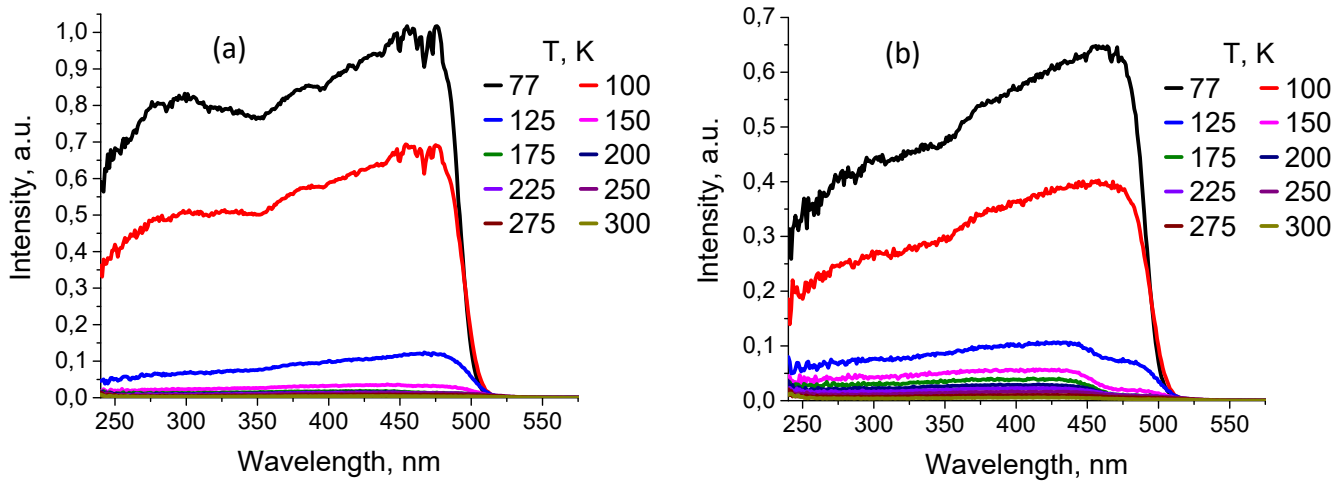


Figure S6. Temperature dependent excitation spectra of **2** recorded for (a) HE emission band (λ_{em} = 600 nm); (b) LE emission band (λ_{em} = 660 nm).

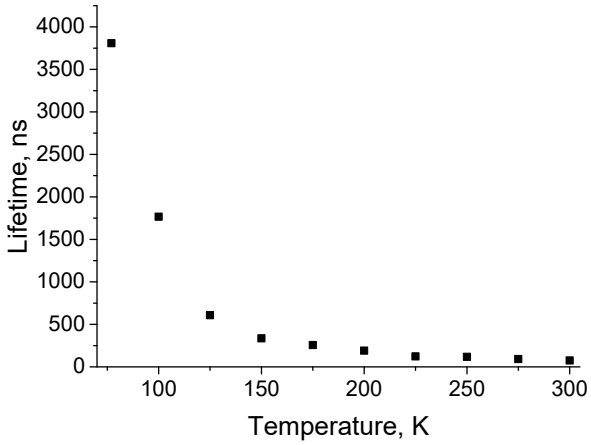


Figure S7. Temperature dependence of the LE emission lifetimes of **2** (λ_{ex} = 390 nm).

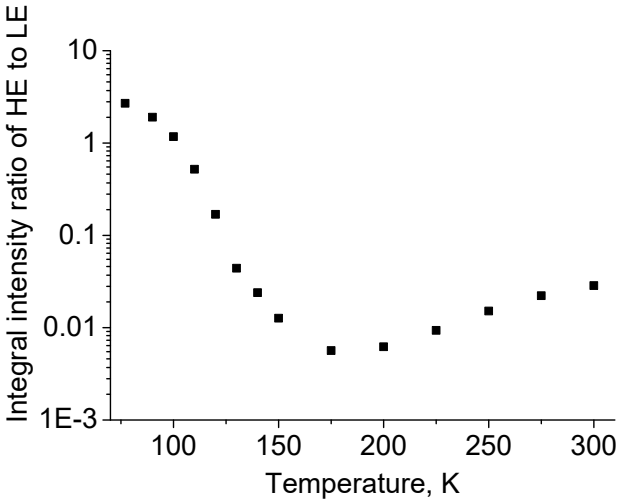


Figure S8. The I_{HE}/I_{LE} integral ratio of **1** as a function of temperature.

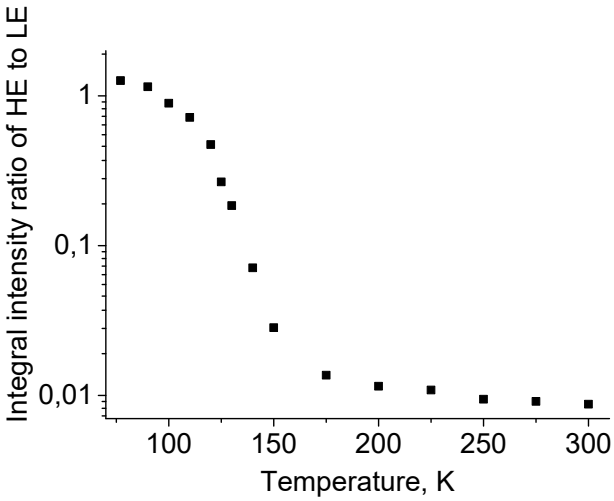
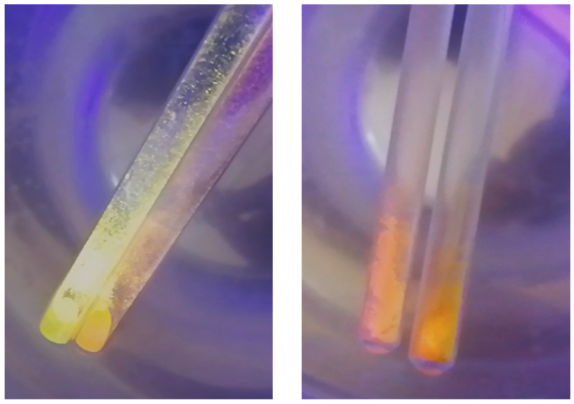


Figure S9. The I_{HE}/I_{LE} integral ratio of **2** as a function of temperature.



Under UV-light, ≈80 K

Under UV-light, ≈300 K

Figure S10. Thermochromic luminescence of **1** (*left*) and **2** (*right*).