Supporting Information for:

Efficient Crystallization Induced Emissive Materials Based on a Simple Push-Pull Molecular Structure

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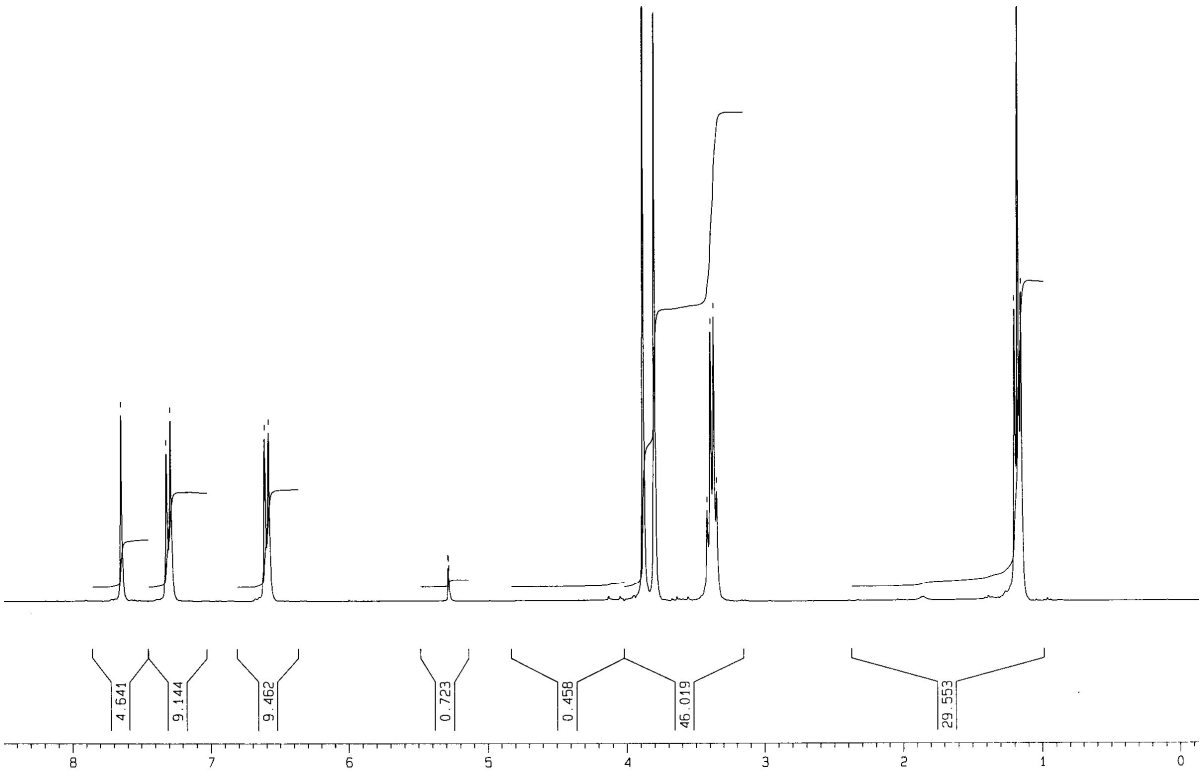

Figure S1. ^{1}H NMR spectrum of compound **3**.

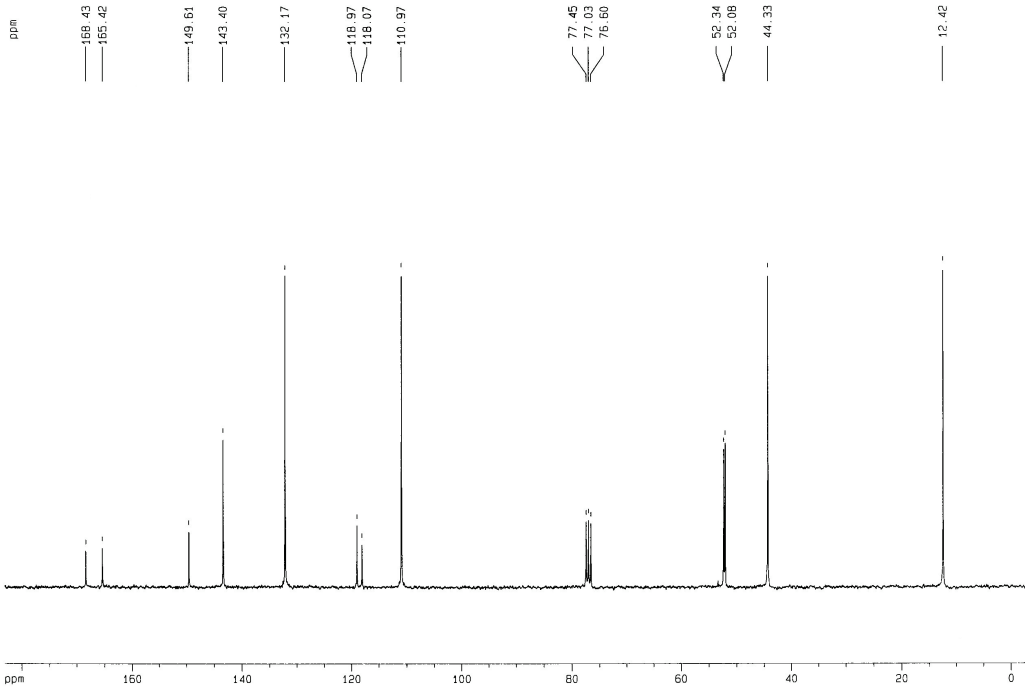

Figure S2 ^{13}C NMR spectrum of compound **3**.

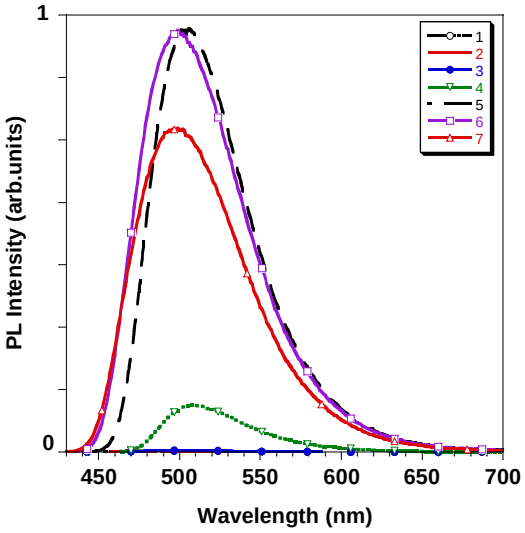

Figure S3. PL spectra of **3** in CH_3OH/water mixtures with increasing water content from 1 to 7.

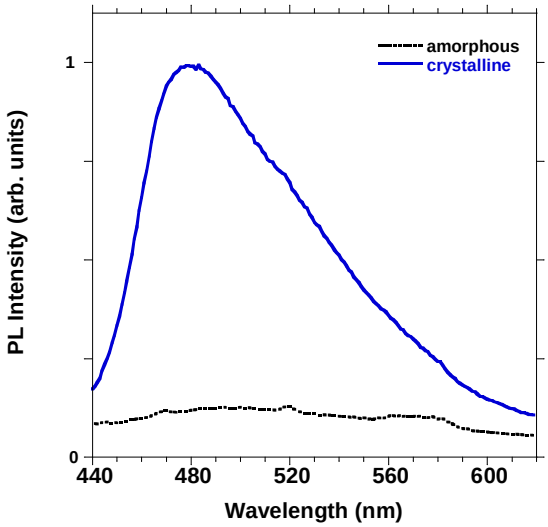

Figure S4. PL spectra of **3** film in the crystalline and amorphous phases excited at 350nm, the spectra are normalized to the crystalline film emission

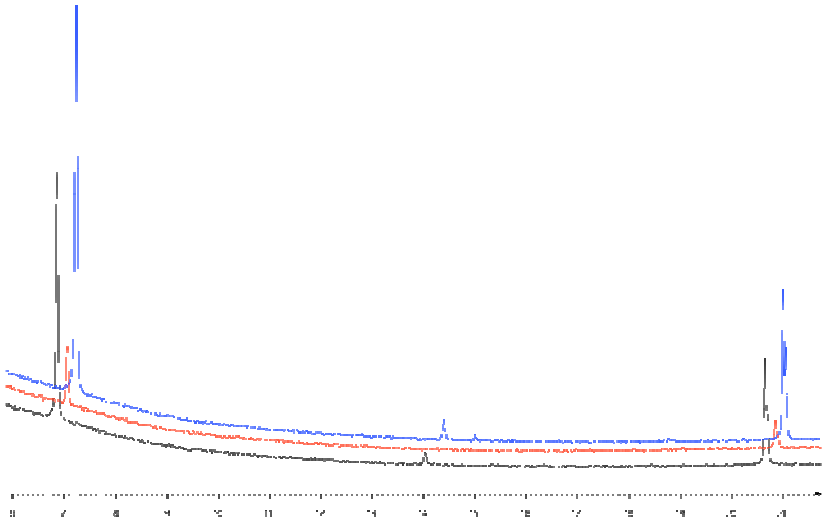

Figure S5 . XRPD patterns, diagonally shifted in order to highlight their relative intensities, of the spin casted films of **1**: black pattern, as casted; red pattern, upon heating and quenching; blue pattern after two weeks. Note that the film are preferentially oriented (the two strongest peaks being the 100 and 300, respectively).

Single crystal data collection, structure solution and refinement.

Crystal samples were mounted on glass fibres in air and collected at RT on a Bruker AXS APEX2 CCD area-detector diffractometer. Graphite-monochromatized Mo-Kα (λ = 0.71073 Å) radiation was used with the generator working at 50 kV and 35 mA. Orientation matrixes were initially obtained from least-squares refinement on ca. 300 reflections measured in three different ω regions, in the range $0 < \theta < 23°$; cell parameters were optimised on the position, determined after integration, of the most accurate reflections. The intensity data were collected in the full sphere (ω scan method); the first 60 frames were recollected to have a monitoring of crystal decay, which was not observed; an empirical absorption correction was applied (SADABS[1]). The structures were solved by direct methods (SIR97)[2] and refined with full-matrix least squares (SHELX97)[3] on F^2 on the basis of the pertinent independent reflection; anisotropic temperature factors were assigned to all non-hydrogenic atoms. Hydrogens were riding on their carbon atoms.

Crystal data for **1**: C14 H17 N O4, Mr = 263.29, monoclinic, space group $P2_1/c$ (No. 14), a = 13.179(3), b = 7.241(2), c = 15.270(4) Å, ß = 101.58(1)°, V = 1427.5(6) $Å^3$, Z = 4, d_{calc} = 1.225 g cm^{-3}, T = 293(2) K, crystal size = 0.19 × 0.04 × 0.04 mm^3, μ = 0.09, MoKα radiation λ= 0.71073 Å. Nominal sample to detector distance 6 cm., 1500 frames (50 s per frame; Δω = 0.5°); Refinement of 176 parameters on 2739 independent reflections out of 14246 measured reflections (Rint = 0.0560, Rσ = 0.0351, 2θ max = 56.0°) led to R1 = 0.0547 (I > 2s(I) , 2138 reflections), wR2 = 0.1743 (all data), and S = 1.043, with the largest peak and hole of 0.22 and -0.25 e $Å^{-3}$.

Crystal data for **2**: C14 H17 N O4, Mr = 263.29, monoclinic, space group $P2_1/c$ (No. 14), a = 14.737(1), b = 7.533(1), c = 15.936(1) Å, ß = 115.27(1)°, V = 1599.9(2) $Å^3$, Z = 4, d_{calc} = 1.21 g cm^{-3}, T = 293(2) K, crystal size = 0.22 × 0.15 × 0.10 mm^3, μ = 0.09, MoKα radiation λ= 0.71073 Å. Nominal sample to detector distance 5 cm., 1500 frames (40 s per frame; Δω = 0.5°); Refinement of 214 parameters on 5125 independent reflections out of 14928 measured reflections (Rint = 0.0221, Rσ = 0.0173, 2θ max = 62.5°) led to R1 = 0.0632 (I > 2s(I), 3232 reflections), wR2 = 0.0959 (all data), and S = 1.035, with the largest peak and hole of 0.50 and -0.27 e $Å^{-3}$.

Crystal data for **3**: C14 H17 N O4, Mr = 263.29, monoclinic, space group C2/c (No. 15), a = 23.263(3), b = 7.821(1), c = 19.649(2) Å, ß = 116.61(1)°, V = 3196.2(7) $Å^3$, Z = 8, d_{calc} = 1.21 g cm^{-3}, T = 293(2) K, crystal size = 0.22 × 0.15 × 0.10 mm^3, μ = 0.09, MoKα radiation λ= 0.71073 Å. Nominal sample to detector distance 5 cm., 1500 frames (90 s per frame; Δω = 0.5°); Refinement of 194 parameters on 4111 independent reflections out of 22714 measured reflections (Rint = 0.0371, Rσ = 0.0280, 2θ max = 57.2°) led to R1 = 0.0464 (I > 2s(I), 2449 reflections), wR2 = 0.0888 (all data), and S = 1.016, with the largest peak and hole of 0.15 and -0.15 e $Å^{-3}$.

Definitions of reported R-indices and weights:

$\mathbf{R_{int} = \Sigma|F_o^2 - F_o^2(mean)|/\Sigma F_o^2}$; $\mathbf{R_\sigma = \Sigma\sigma(F_o^2)/\Sigma F_o^2}$
$\mathbf{R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|}$ $\mathbf{wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{½}}$
Goodness of fit $\mathbf{GoF = \{S/(n-p)\}^{½} = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{½}}$ where **n** and **p** are the number of observations and refined parameters, respectively.
$\mathbf{w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]}$ where $\mathbf{P = [2F_c^2 + Max(F_o^2, 0)]/3}$

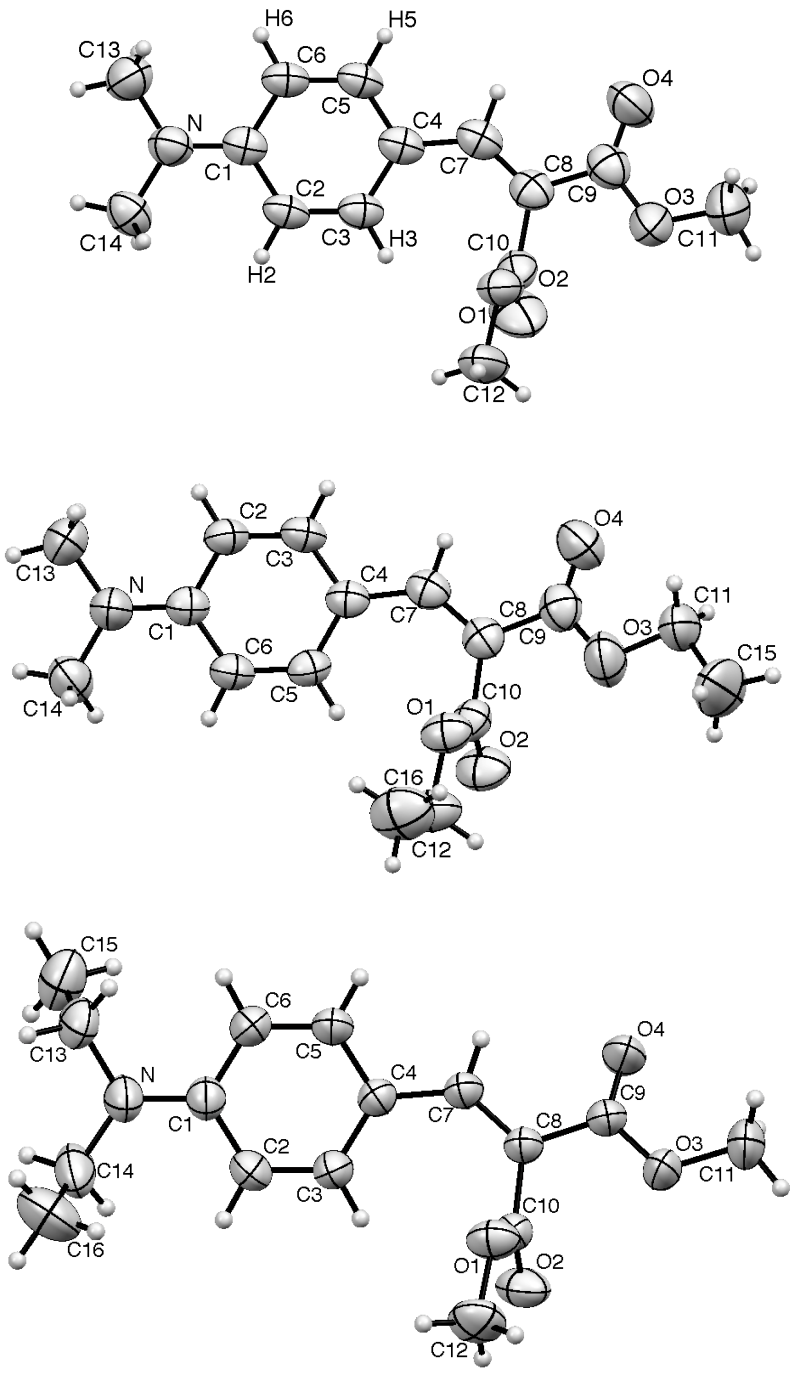

Figure S6. ORTEP view of **1-3** (the ellipsoid have been at the 50% probability level)

1 Sheldrick, G. M. (1996) *SADABS*, University of Göttingen, Germany, to be published.
2 A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, J. Appl. Cryst. 1999, **32**, 115.
3 G. M. Sheldrick, SHELX-97 Programs for Crystal Structure Analysis (Release 97-2), University of Göttingen (Germany), 1997.