# Supporting Information

# Luminescence Properties of 1,8-naphthalimide Derivatives in Solution, in Their Crystals and in Co-Crystals: Towards Room Temperature Phosphorescence from Organic Materials

*Barbara Ventura,*[§] Alessio Bertocco,[‡] Dario Braga,[‡] Luca Catalano,[‡] Simone d'Agostino,[‡] Fabrizia Grepioni*[‡] and Paola Taddei*[¤]*

[§] Istituto ISOF-CNR, Via P. Gobetti 101, 40129 Bologna, Italy.

[‡] Dipartimento di Chimica G. Ciamician, Università di Bologna, Via F. Selmi 2, 40126 Bologna

[¤] Dipartimento di Scienze Biomediche e Neuromotorie, Università di Bologna, Via Belmeloro 8/2, 40126 Bologna

**Table of Contents**

**Absorption and luminescence data in solution**

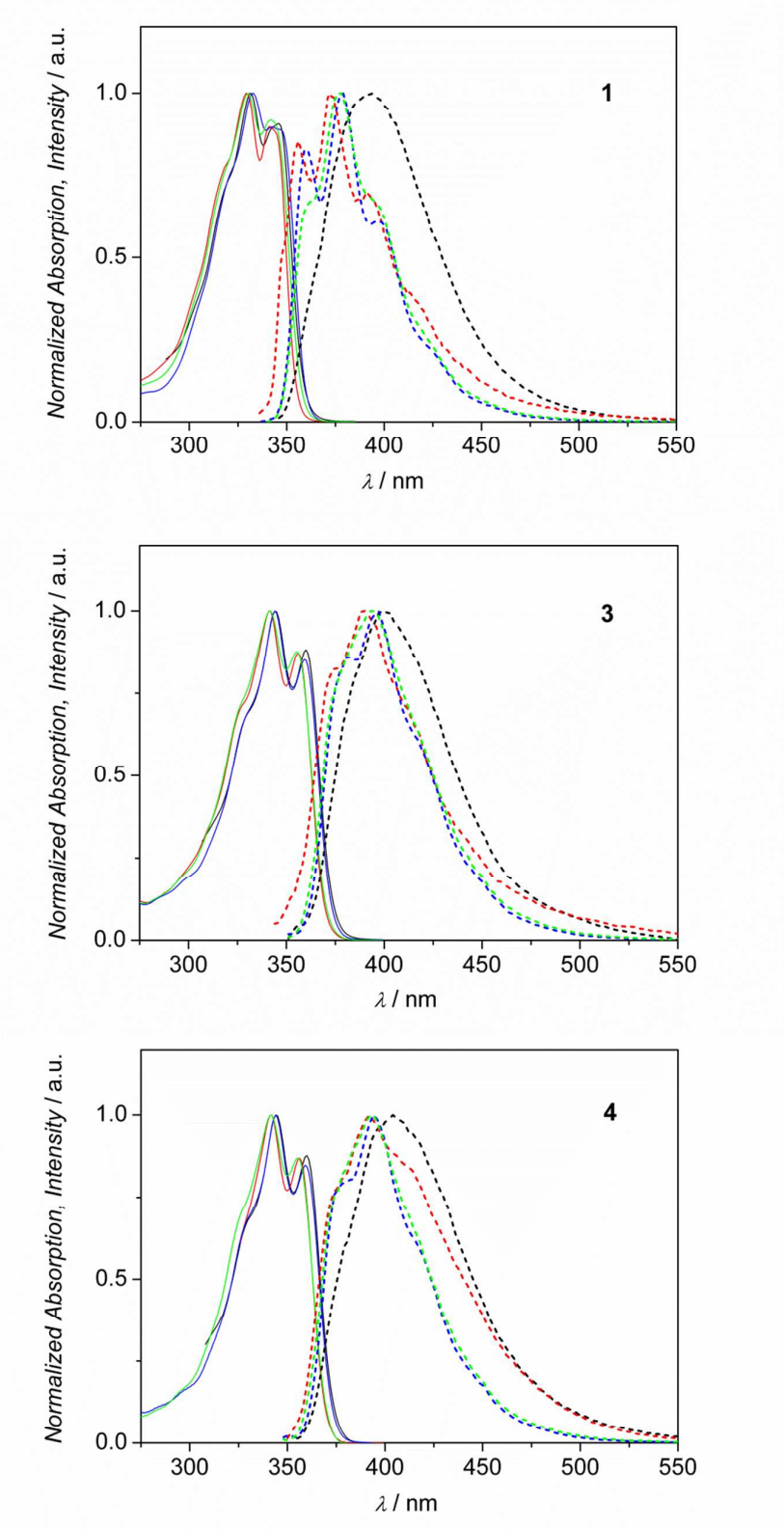


**Figure S1**. Absorption (full lines) and emission (dotted lines) spectra of **1**, **3**, and **4** in TOL (black), THF (red), DCM (blue) and ACN (green). Excitation at 330 nm for **1** and at 340 nm for **3** and **4**.

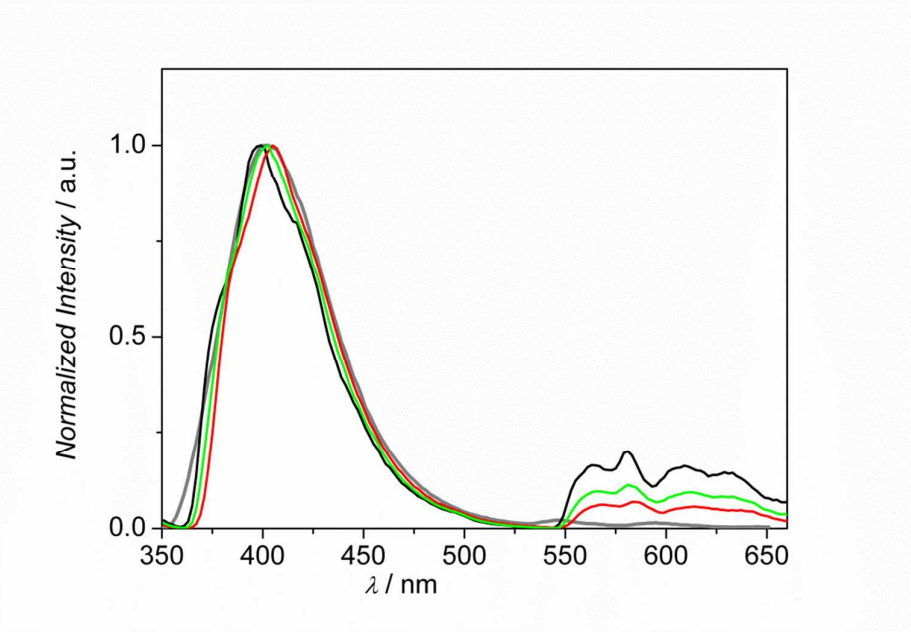


**Figure S2**. Luminescence spectra of **1** (gray), **2** (black), **3** (red) and **4** (green) in TOL at 77 K. Excitation at 330 nm. The spectra are normalized on the maximum of fluorescence.

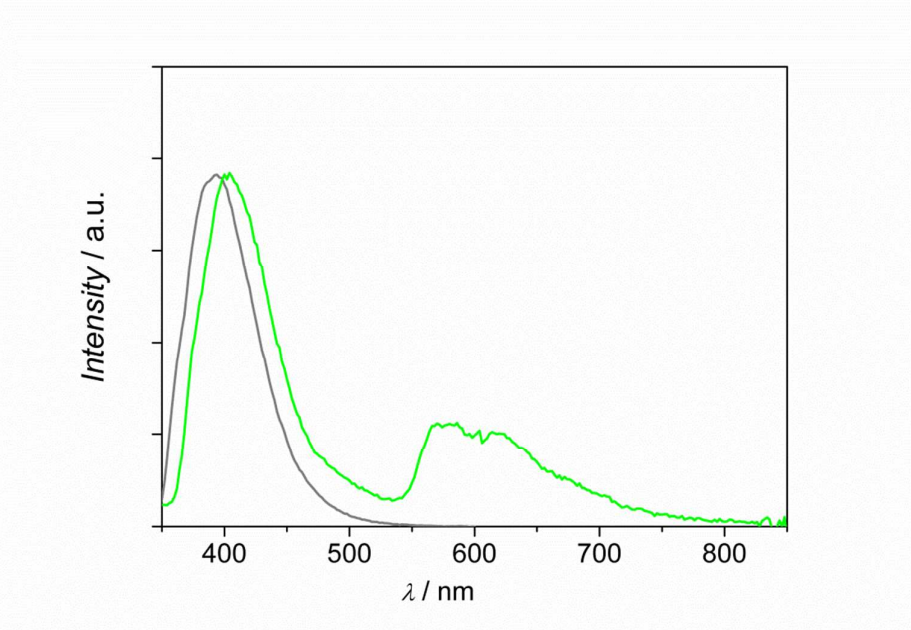


**Figure S3**. Luminescence spectra of **1** (grey) and **4** (green) in air-free TOL at room temperature. Excitation at 310 nm. The spectra are normalized on the maximum of fluorescence intensity.

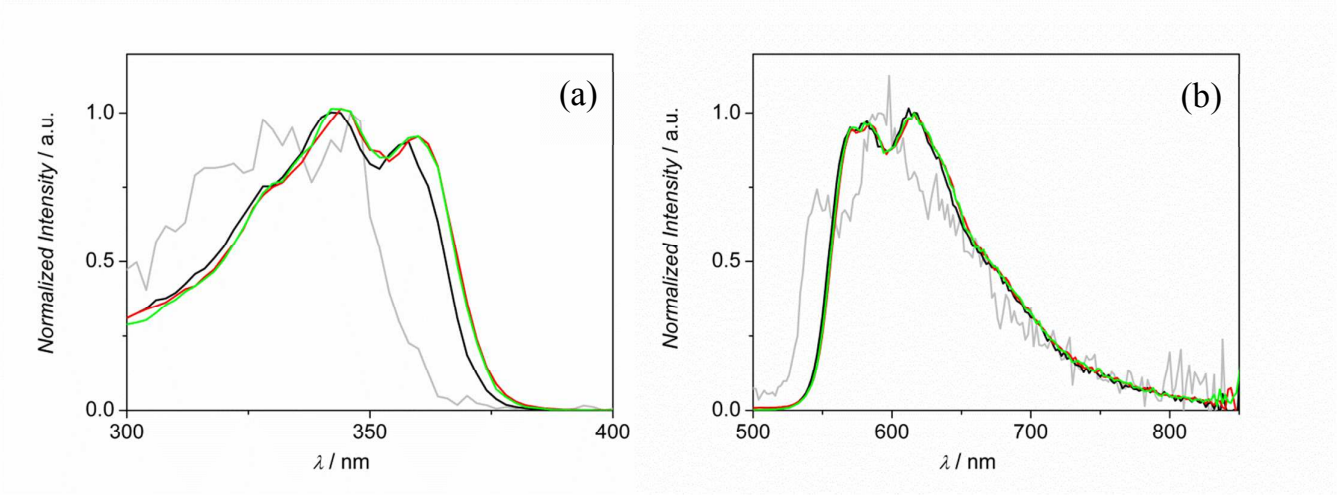


**Figure S4**. Excitation (a) and phosphorescence (b) spectra of **1** (gray), **2** (black), **3** (red) and **4** (green) in air-free TOL at room temperature, registered in gated mode. Gating parameters: delay: 0.1 ms, gate: 0.2-0.5 ms. In (a) $\lambda_{em}$ = 600 nm; in (b) $\lambda_{exc}$ = 340 nm.

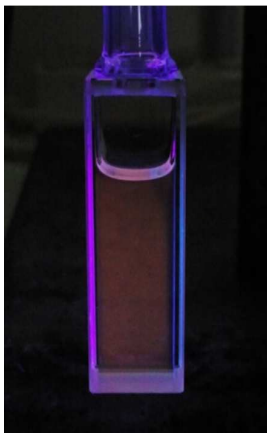

**Figure S5**. Picture of an air-free TOL solution of **4** upon UV irradiation (UVGL-55 lamp). $A_{340}$ = 0.080.

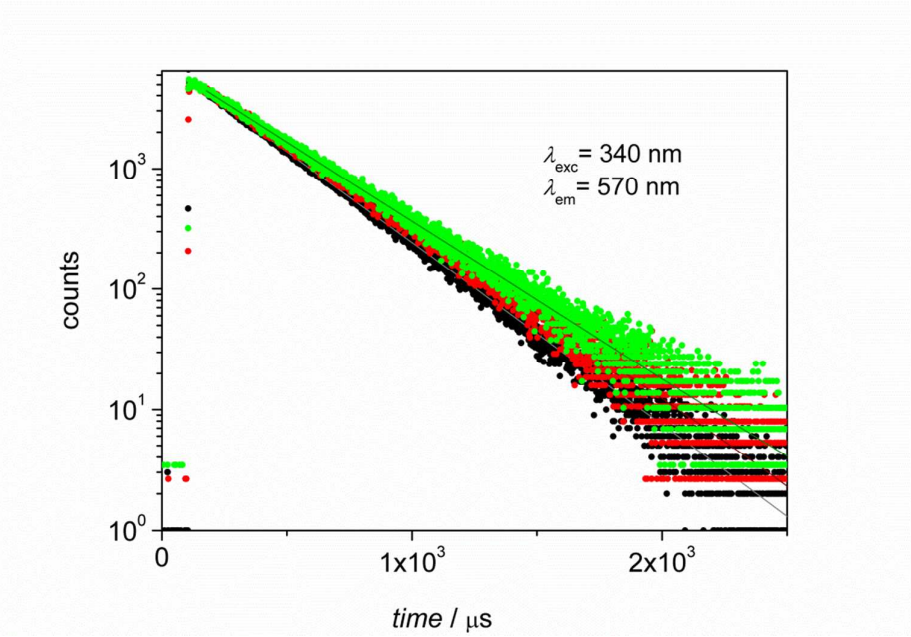


**Figure S6**. Phosphorescence decays, on a semi-log scale, of **2** (black), **3** (red) and **4** (green) in air-free TOL at room temperature and mono-exponential fittings.

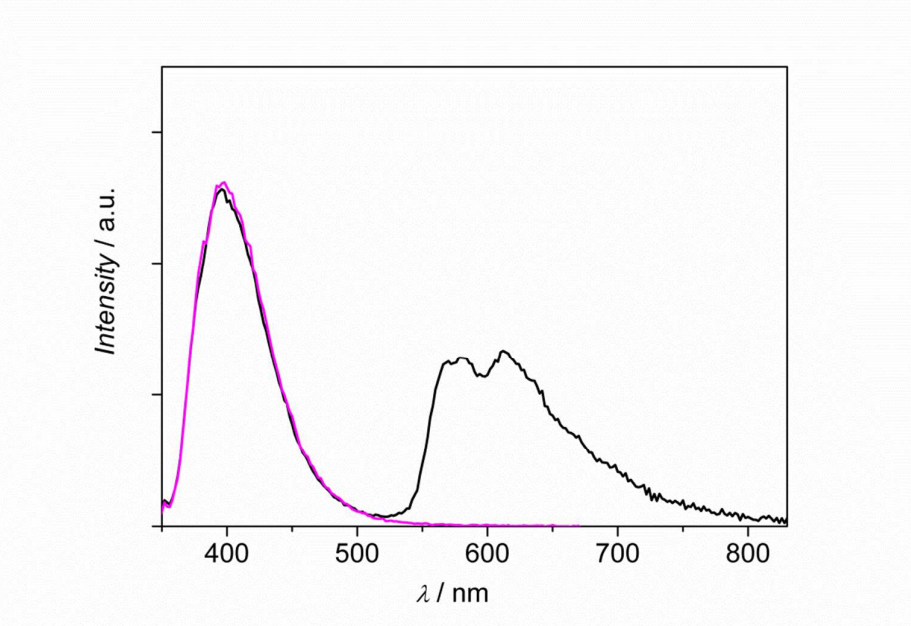


**Figure S7**. Luminescence spectra from optically matched TOL solutions of **2** in air-free solution (black) and in air-equilibrated solution (pink). Excitation at 340 nm, $A_{340}$ = 0.080.

## IR Spectra

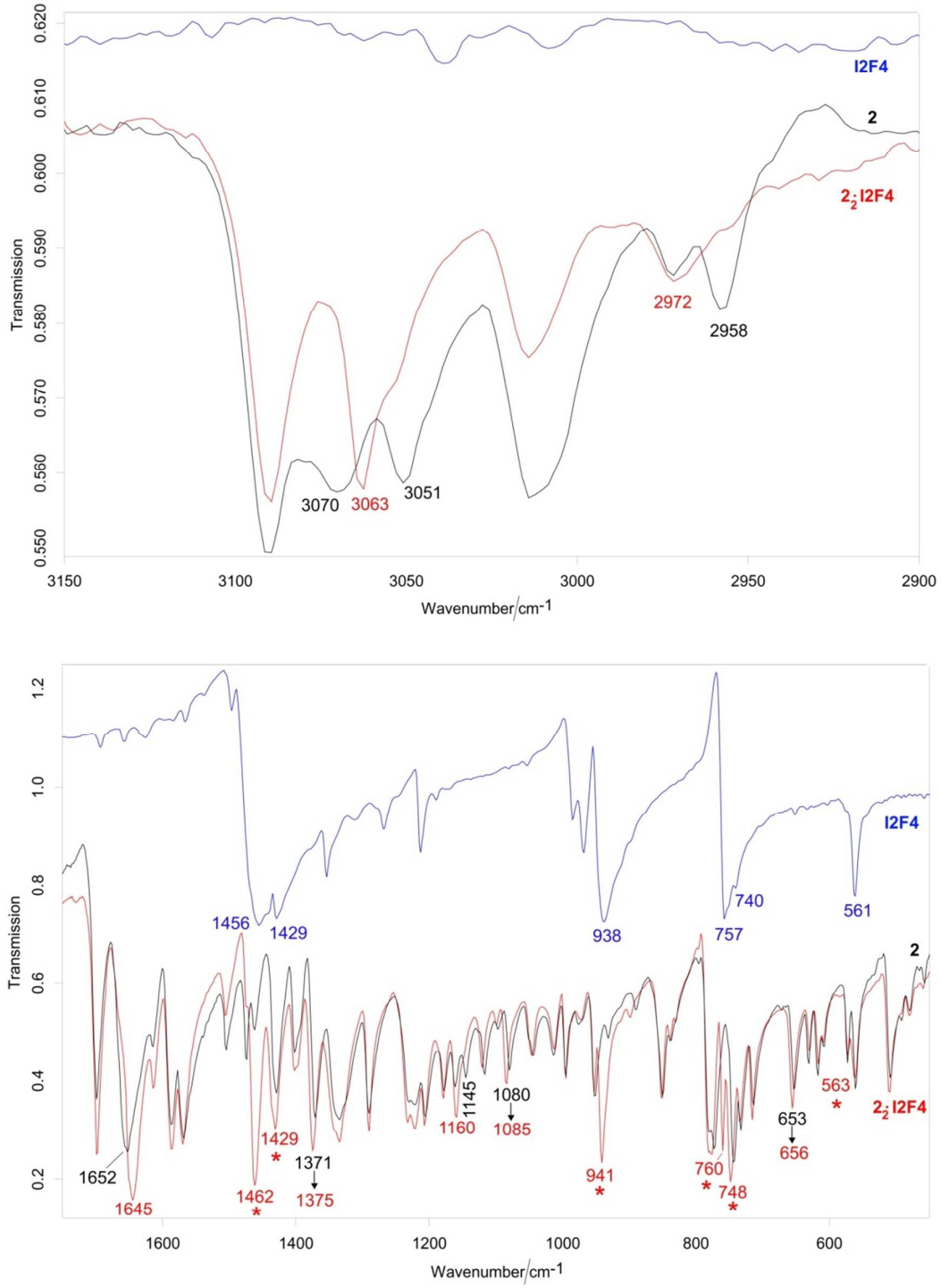


**Figure S8**. 3150-2900 $cm^{-1}$ (top) and 1750-450 $cm^{-1}$ (bottom) IR spectra of **2** (black), **I2F4** (blue) and **$2_2$·I2F4** (red). The bands of **I2F4** are indicated with an asterisk.

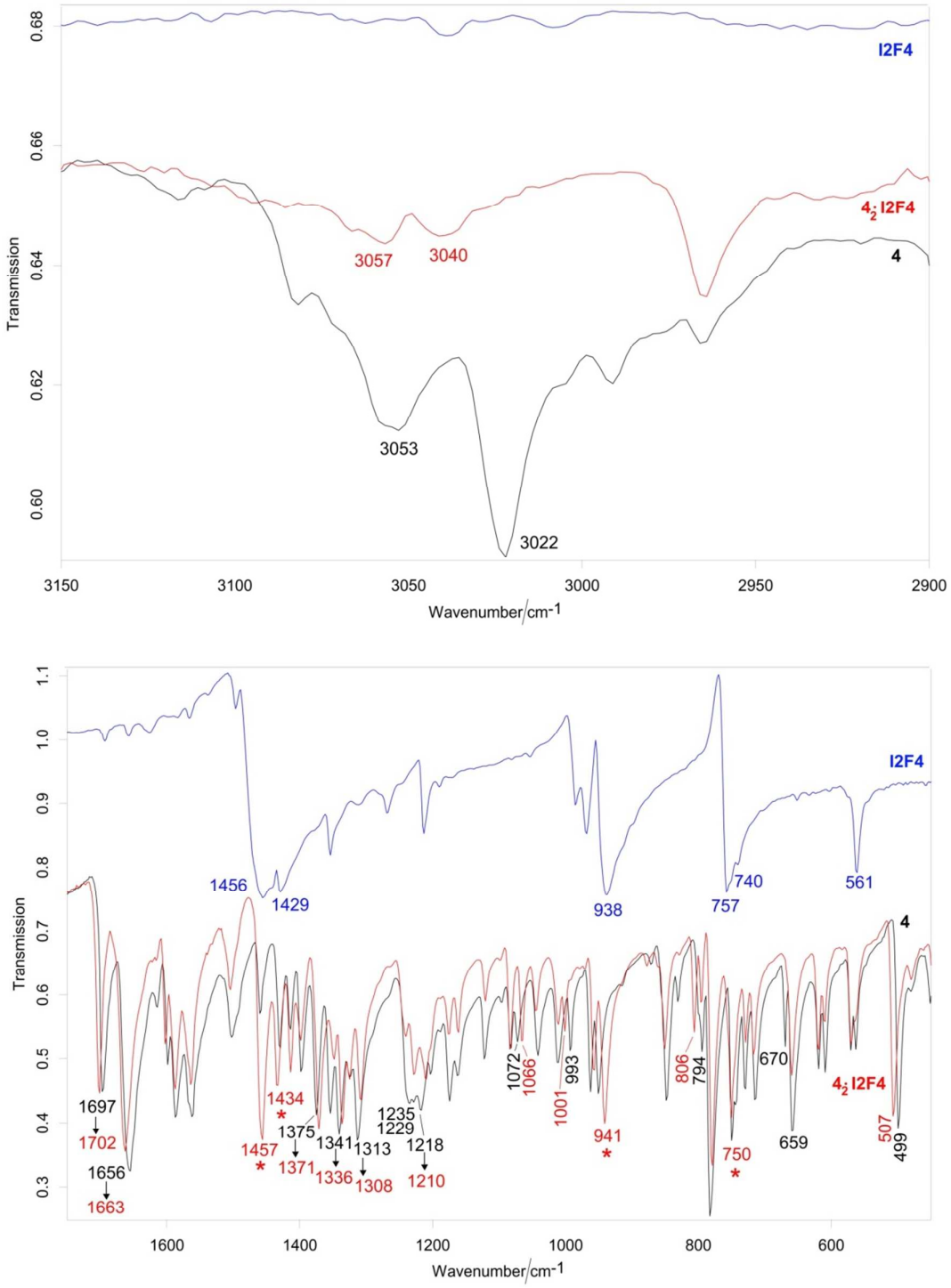


**Figure S9**. 3150-2900 $cm^{-1}$ (top) and 1750-450 $cm^{-1}$ (bottom) IR spectra of **4** (black), **I2F4** (blue) and **$4_2$·I2F4** (red). The bands of I2F4 are indicated with an asterisk.

**Absorption and luminescence data in the solid state**

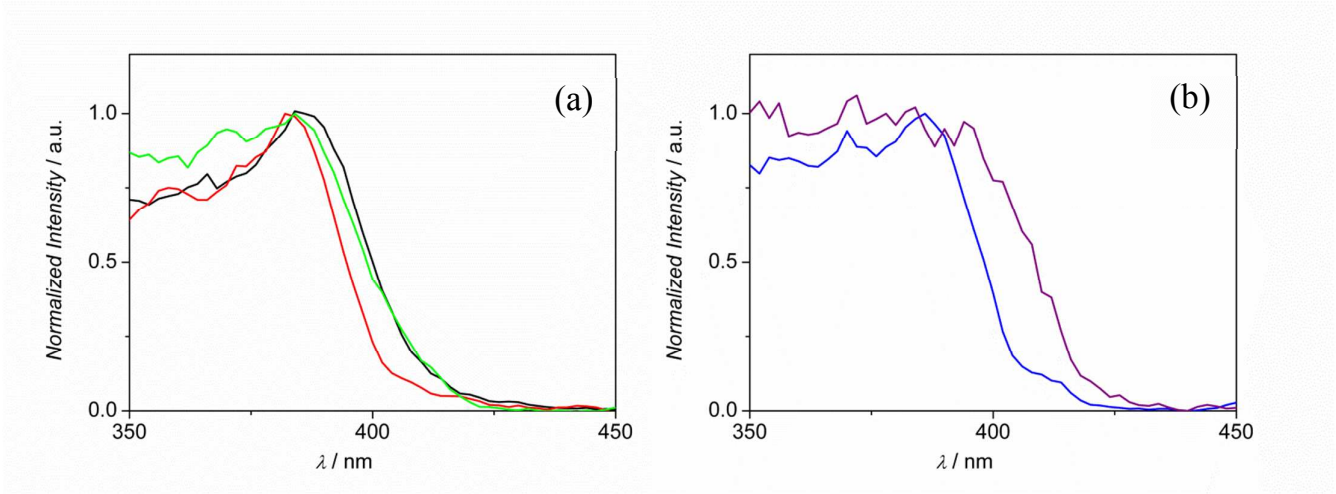


**Figure S10**. Excitation spectra collected on phosphorescence maxima of (a) **2** (black), **3** (red), and **4** (green) and (b) **$2_2$·I2F4** (blue) and **$4_2$·I2F4** (purple) in the solid state. Gating parameters: delay: 0.1 ms, gate: 2-3 ms.

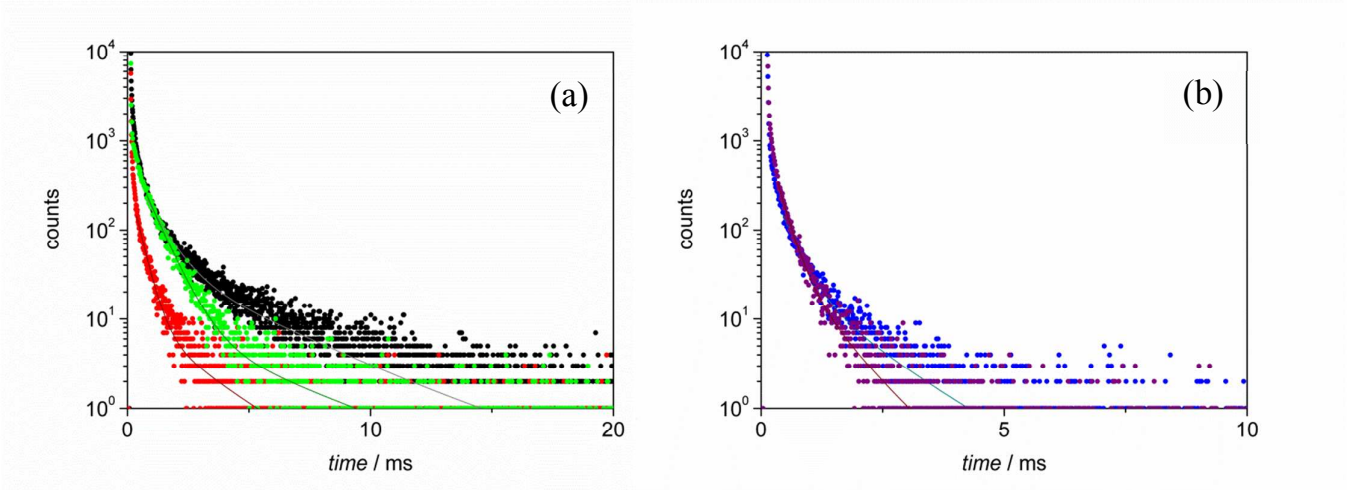


**Figure S11**. Phosphorescence decays, on a semi-log scale, of (a) **2** (black), **3** (red), and **4** (green) and (b) **$2_2$·I2F4** (blue) and **$4_2$·I2F4** (purple) in the solid state at room temperature, and bi-exponential fittings.

**X-ray data**

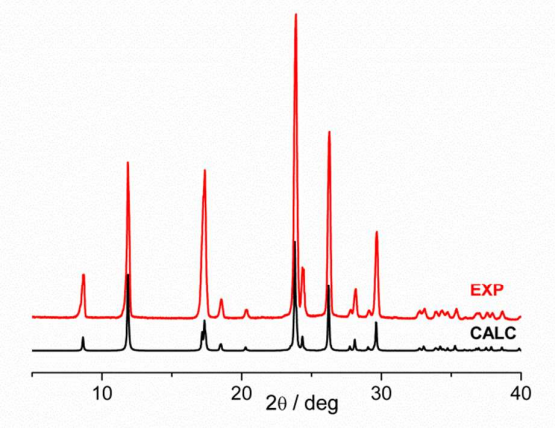


**Figure S12.** Comparison of calculated (on the basis of single crystal data) and measured X-ray powder patterns for compound **1**.

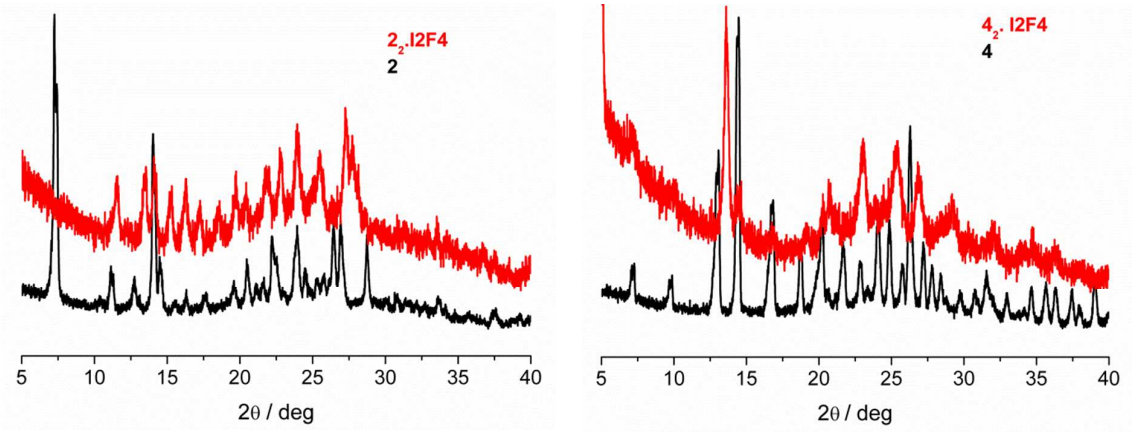


**Figure S13.** Comparison of experimental X-ray powder patterns for compound **2** and **4** and the relative co-crystals with the **I2F4** co-former, namely **$2_2$·I2F4** and **$4_2$·I2F4**, left and right respectively.

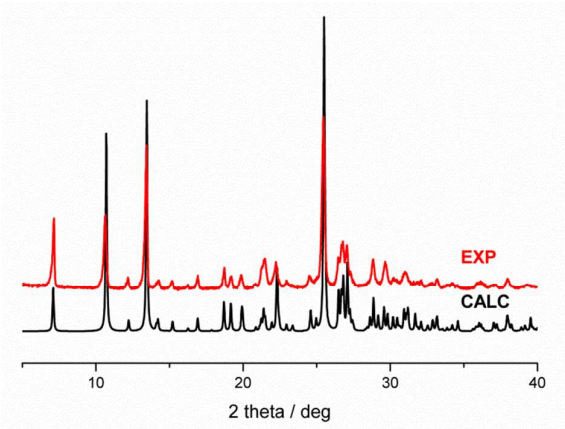


**Figure S14.** Comparison of calculated (on the basis of single crystal data) and measured X-ray powder patterns for compound **3**.

**Table S1**. Crystallographic data and details of measurements for compound **3**.

| | **3** |
|---|---|
| Formula | $C_{18}H_{11}BrN_2O_2$ |
| fw | 367.20 |
| Cryst. System | Triclinic |
| Space group | P-1 |
| Z | 2 |
| a (Å) | 7.0727(8) |
| b (Å) | 8.796 (1) |
| c (Å) | 12.650 (1) |
| α (deg) | 92.803(9) |
| β (deg) | 98.280(9) |
| γ (deg) | 109.299(10) |
| V ($Å^3$) | 731.06(1) |
| $D_{calc}$ ($Mg/m^3$) | 1.668 |
| μ ($mm^{-1}$) | 2.823 |
| Measd reflns | 4785 |
| Indep reflns | 2819 |
| $R_1$[on $F_0^2$, $I>2\sigma(I)$] | 0.1040 |
| $wR_2$ (all data) | 0.3016 |