Aggregation-induced enhanced green light emission from a simple donor-π-acceptor (D-π-A) material: A structure-property relationship study

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Supporting Information
Fig. S1 $^1$H NMR spectrum of A1.

Fig. S2 $^{13}$C NMR spectrum of A1.

Fig. S3 $^1$H NMR spectrum of A2.
Fig. S4 \(^{13}\)C NMR spectrum of A2.

**FT-IR**

Fig. S5 FT-IR spectrum of A1.

Fig. S6 FT-IR spectrum of A2.
Single crystal growth and crystallographic data

The single crystals of A1 and A2 were grown from the saturated 1:1 acetone–methanol and 1:1 acetone–acetonitrile solution by slow evaporation technique, respectively. For this purpose, saturated solutions of compounds were kept at room temperature for slow evaporation of solvent. After a couple of days, small crystals were harvested and used for X-ray analysis.

Table S1 Structural parameters for A1 and A2

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<th>A1</th>
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<tbody>
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<td>Empirical formula</td>
<td>C₁₂H₁₂N₂O₃</td>
<td>C₁₁H₁₀N₂O₂</td>
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<tr>
<td>Mᵣ</td>
<td>232.24</td>
<td>202.21</td>
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<tr>
<td>Crystal size (mm)</td>
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<td>0.4×0.3×0.2</td>
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<tr>
<td>Crystal system</td>
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<tr>
<td>Space group</td>
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<td>P ₂/c</td>
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<tr>
<td>b [Å]</td>
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<td>T [K]</td>
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Table S2 Bond Lengths (Å) and Bond Angles (deg) in the Structures Studied.

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A1

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Absorption and fluorescence spectra

**Fig. S7** (a) Absorption spectra of A1, (b) absorption spectra of A2, (c) fluorescence spectra of A1 and (d) fluorescence spectra of A2 in different solvents with molar concentration $1.0 \times 10^{-5}$ M.

**Quantum yield**

The relative fluorescence quantum yield ($\Phi_f$) of compounds were calculated in different organic solvents using widely spread method introduced by Parker and Rees (equation 1),

$$\Phi_f = \frac{\phi_s f_s(\lambda_{ex}) \int_{\lambda_{em}} F(\lambda_{em}) n_i^2}{\phi_i f_i(\lambda_{ex}) \int_{\lambda_{em}} F(\lambda_{em}) n_s^2}$$

where $i$ stands for the sample and $s$ for standard; $n$ is the refractive index of the solvent used, term $\int_{\lambda_{em}} F(\lambda_{em})$ represents the area under the fluorescence curve and $f_i(\lambda_{ex}) = 1 - 10^{-Ax(\lambda_{ex})}$; where $Ax$ is the absorbance. Anthracene has been used as a reference material for the calculation of relative quantum yield.
Differential thermal analysis (DTA) and activation energy calculation

Fig. S9 (a) DTA curve of compounds A1 and A2, (b) Thermal activation energy plot of A1 and (c) Thermal activation energy plot of A2.

The energy of activation ($E_a$) associated with each stage of decomposition is given by the equation:

$$\ln \left[ \ln \left( \frac{1}{y} \right) \right] = \left( - \frac{E_a}{R} \right) \frac{1}{T} + \text{Constant}$$

Where $y = \frac{(W_i-W_\infty)}{(W_o-W_\infty)}$ is the fraction of the number of initial molecules not yet decomposed, $R$ is the gas constant, $T$ is the absolute temperature, $W_i$ is the weight at any time $t$, $W_\infty$ is the weight at infinite time. The energy of activation may be computed from the slope of the $\ln[\ln(1/y)]$ vs. $1/T$ plot which results a straight line. The plot is given in Fig. S 9b and 9c.

References
