

Supporting Information for:

A Highly Fluorescent PN-Heterocycle-fused Pyrene Derivative with Strong Self-dimerization through Hydrogen Bonding

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Additional Crystallographic Figures

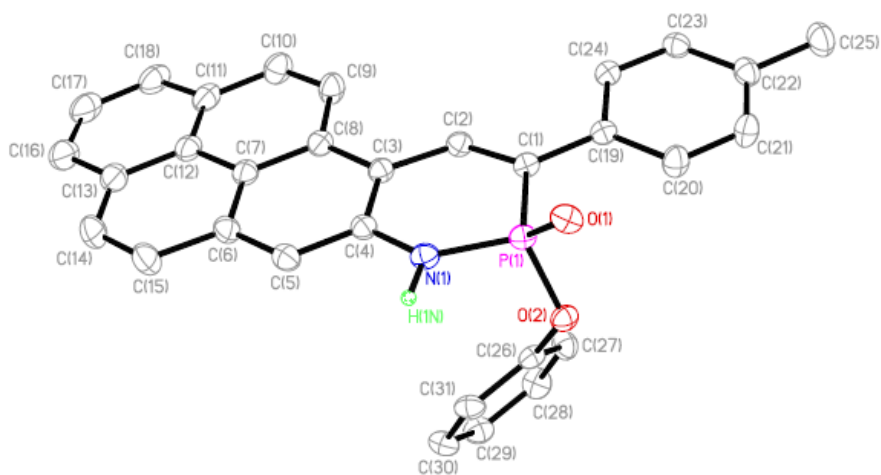


Figure S1. ORTEP drawing of PN-fused pyrene **2**; thermal ellipsoids drawn at 30% probability. Crystals grown from slow layering of pentane into a concentrated solution of **2** in chloroform.

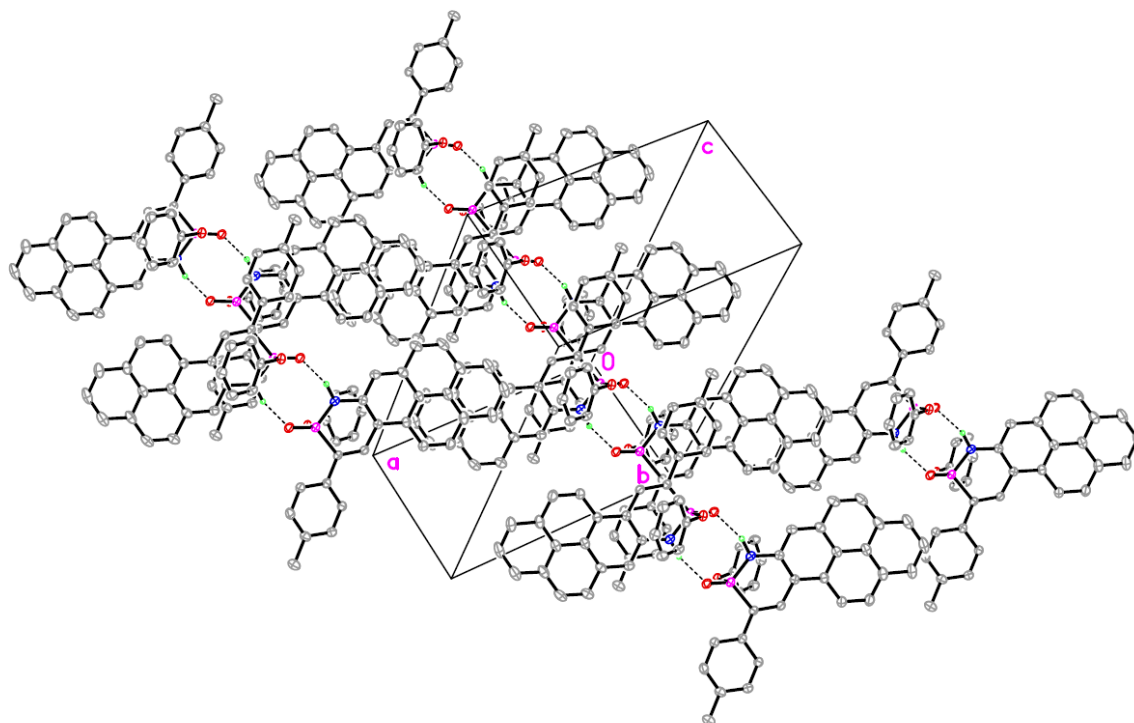


Figure S2. ORTEP drawing of the crystal packing of **2**. Crystals grown from slow layering of pentane into a concentrated solution of **2** in chloroform.

Photophysical Studies in Different Solvents and the Solid-state

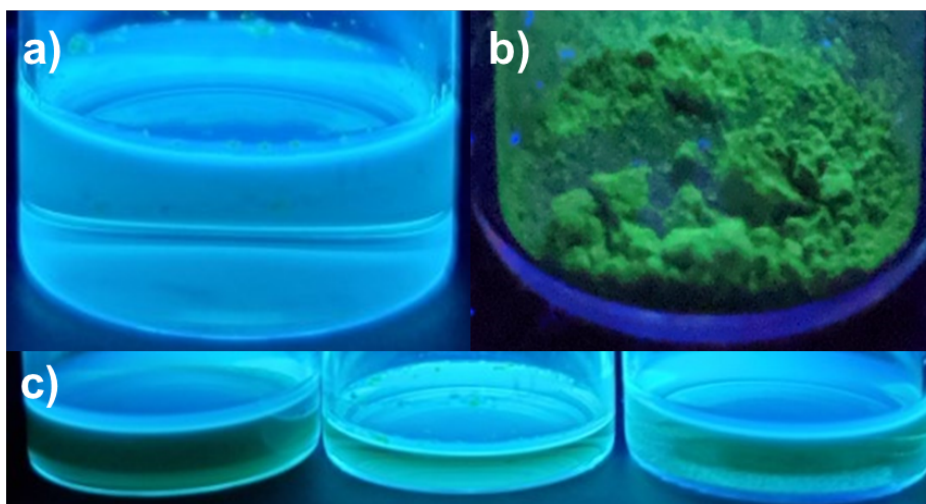


Figure S3. Fluorescence images of **2** in a) chloroform (*ca.* 1 μ M), b) the solid state, and c) (left to right) toluene, chloroform, and methanol at *ca.* 4 mM in concentration. All samples were excited at 365 nm.

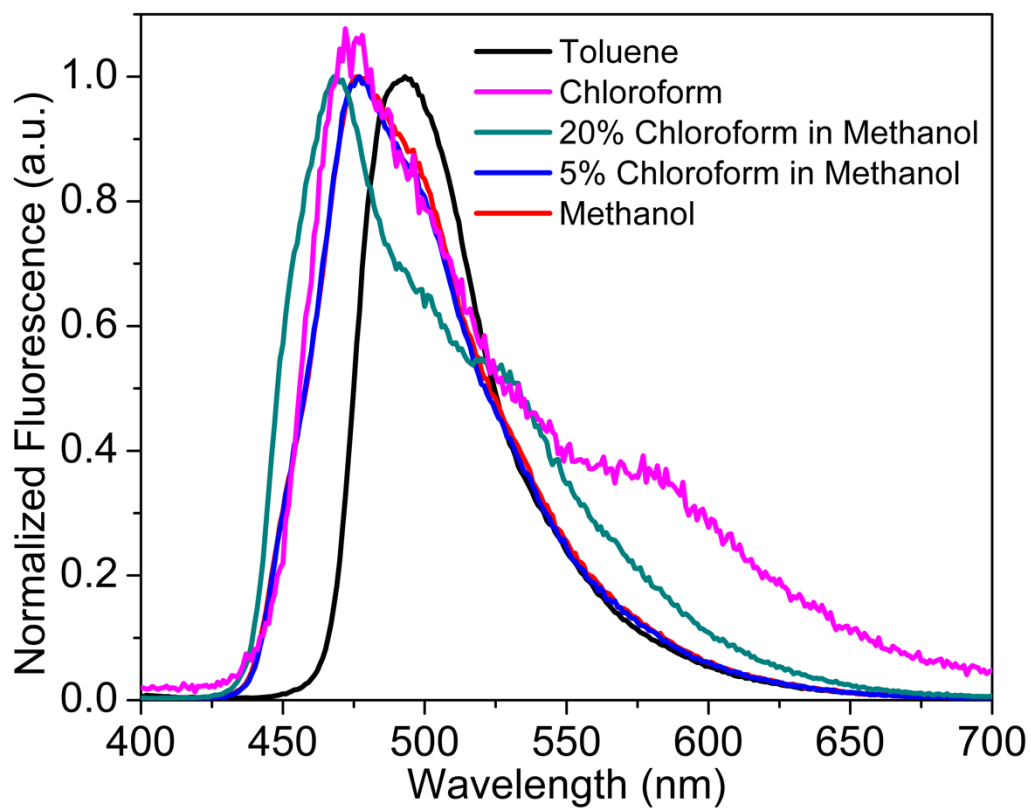


Figure S4. Fluorescence spectra of 4 mM solutions of **2** in a variety of solvents. Samples excited at 365 nm.

Chemical structure of 1-(4-ethynylphenyl)-5-nitro-9H-fluoren-3-one is shown above the spectrum.

¹H NMR spectrum (CDCl₃) showing peaks in the aromatic region (7.2-8.8 ppm) and aliphatic region (1.4-2.5 ppm). Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
8.76, 8.74, 8.73, 8.29, 8.27, 8.26, 8.24, 8.16, 8.14, 8.13, 8.11, 8.05, 8.03, 7.68, 7.67	1.04, 1.00, 3.07, 1.35, 0.85, 1.06, 1.99, 2.04
2.44, 2.44, 2.44	3.00
1.44, 1.44, 1.44	3.00

Chemical structure of 1-(4-methylphenyl)-2-nitro-3-phenylacetylene is shown above the spectrum.

Chemical Shift (ppm)

150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

147.72 146.79 138.59 137.11 136.11 132.11 131.95 131.65 130.65 130.39 130.29 130.11 129.11 128.01 127.30 126.89 126.65 126.15 125.65 119.93 119.85 112.15 103.18 83.41 77.38 77.37 21.85

S4

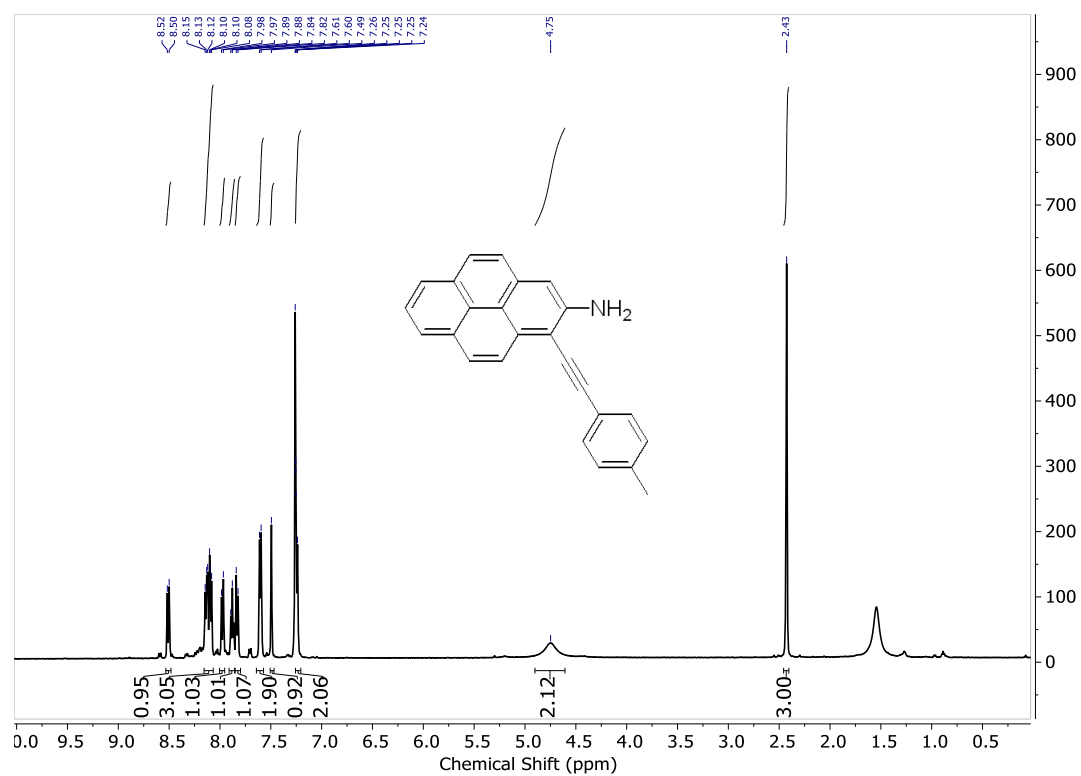


Figure S7. ¹H NMR spectrum of **5** in CDCl₃.

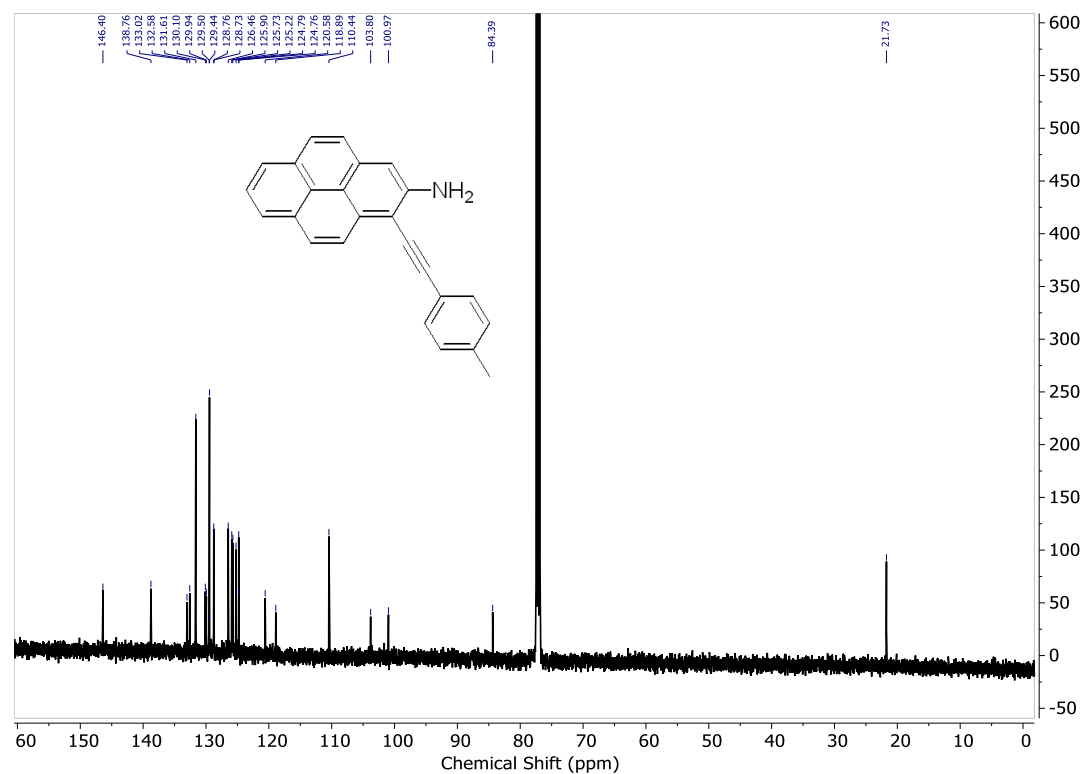


Figure S8. ¹³C NMR spectrum of **5** in CDCl₃.

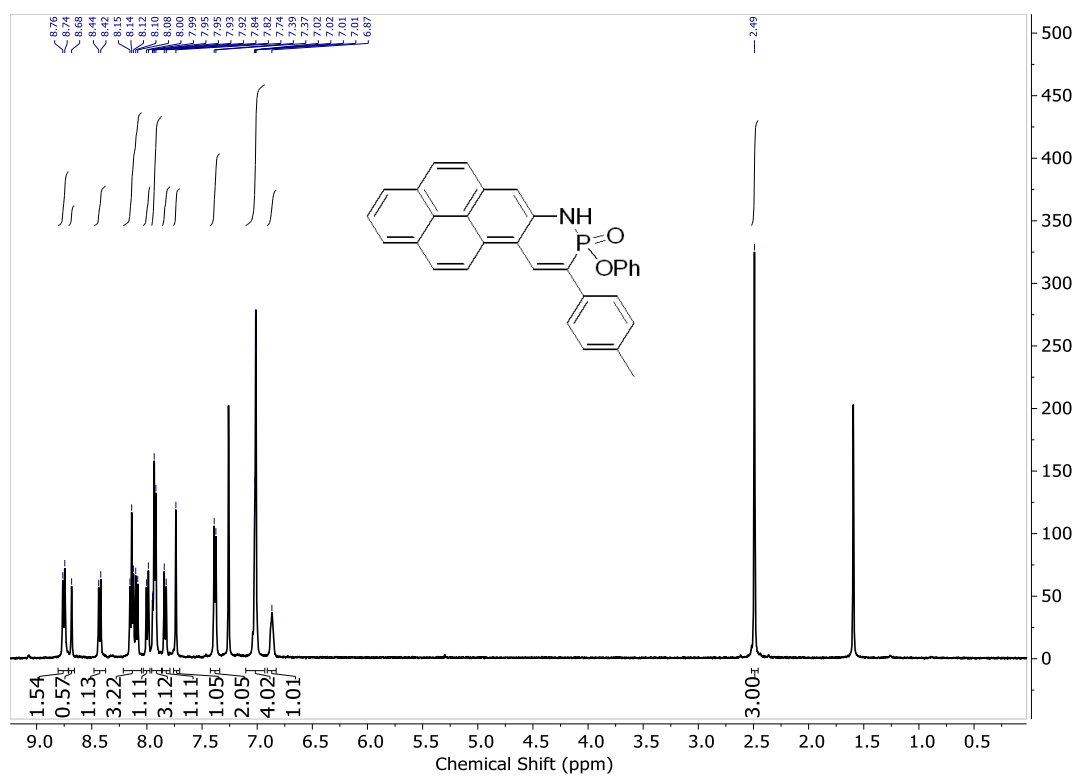


Figure S9. ^1H NMR spectrum of **2** in CDCl_3 .

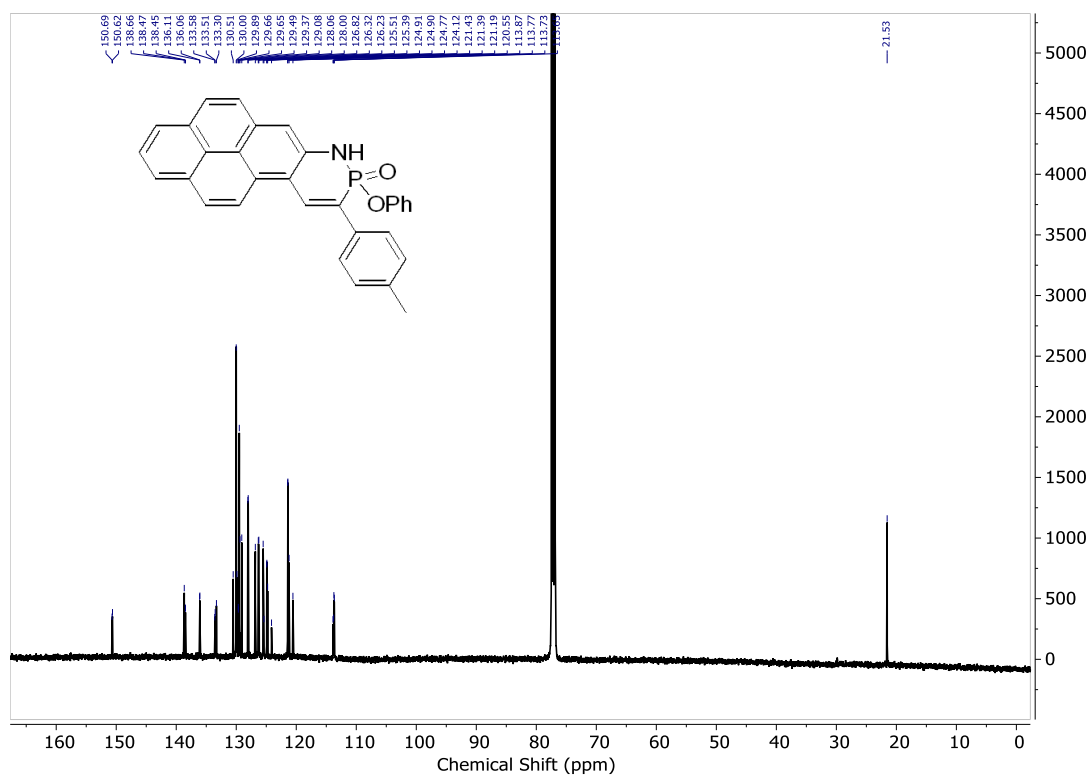


Figure S10. ^{13}C NMR spectrum of **2** in CDCl_3 .

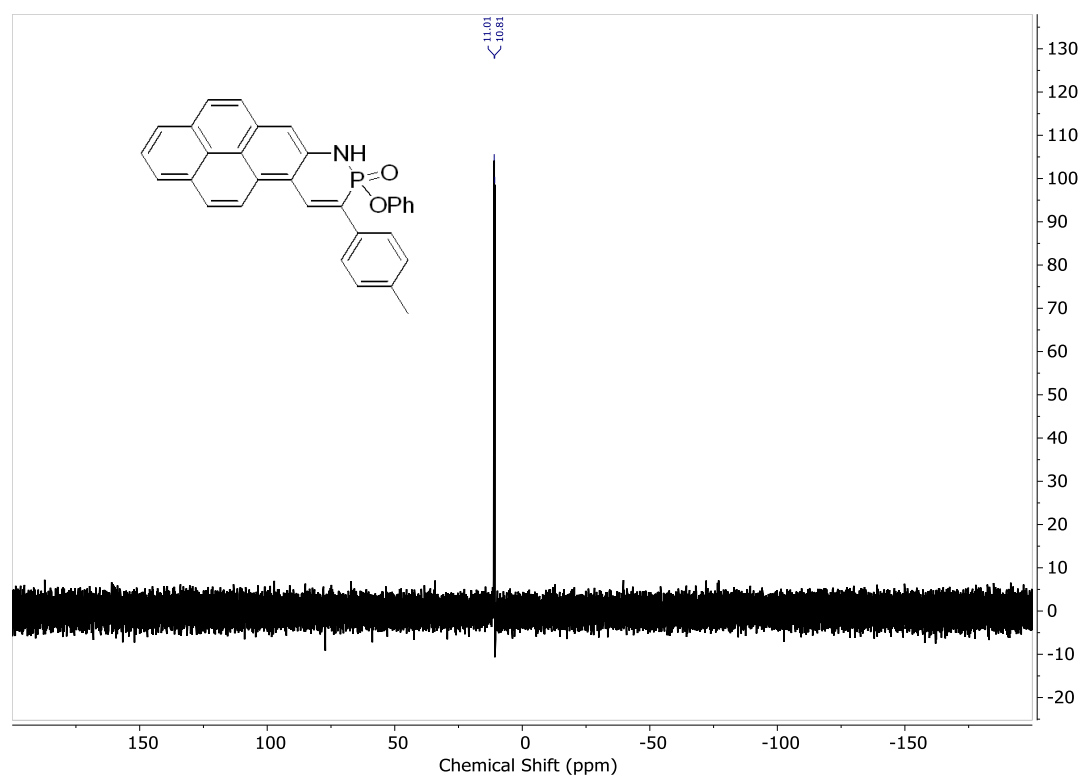


Figure S11. ^{31}P NMR spectrum of **2** in CDCl_3 .