

Supplementary Materials

Solid-state highly efficient DR mono and poly-dicyano-phenylenevinylene fluorophores

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Table S1. Crystallographic data and structural refinement details of CN-PV-NHMe.

Empirical formula	C ₃₅ H ₄₀ N ₄ O ₂
Formula weight	548.71
Temperature (K)	173(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	C 2/c
<i>a</i> (Å)	25.330(7)
<i>b</i> (Å)	16.719(4)
<i>c</i> (Å)	14.804(3)
β (°)	97.269(18)
Volume (Å ³)	6219(3)
<i>Z</i>	8
<i>D</i> _{calc} (Mg/m ³)	1.172
μ (mm ⁻¹)	0.073
<i>F</i> (000)	2352
Crystal size (mm)	0.40 × 0.10 × 0.07
θ range for data collection (°)	2.720 to 25.013
Limiting indices	-30 ≤ <i>h</i> ≤ 30, -19 ≤ <i>k</i> ≤ 19, -17 ≤ <i>l</i> ≤ 16
Reflections collected / unique	27781 / 5463 [<i>R</i> (int) = 0.2470]
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	5463 / 200 / 443
Goodness-of-fit on <i>F</i> ²	1.015
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0833, <i>wR</i> ₂ = 0.1817
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.2390, <i>wR</i> ₂ = 0.2521
Largest diff. peak / hole (e·Å ⁻³)	0.242 / -0.240

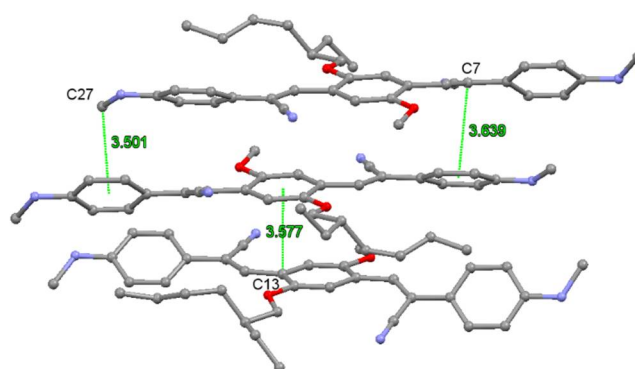


Figure S1. Partial packing of CN-PV-NHMe with shortest distances involving aromatic centroids reported as green dashed lines. Ball-and-stick style, H atoms are not drawn for clarity.

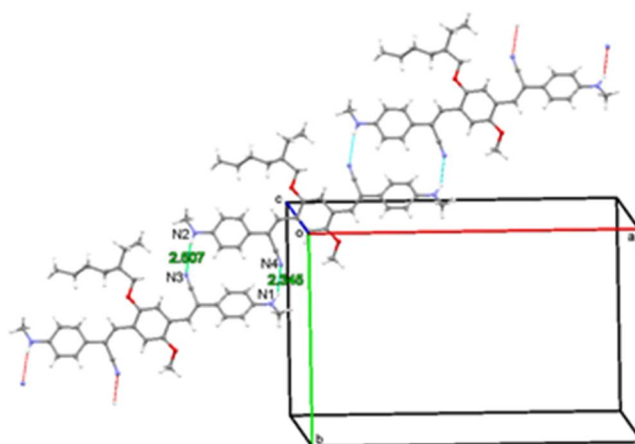


Figure S2. Molecular ribbon of CN-PV-NHMe propagating in the (1 -1 0) direction. Inter-molecular NH...N bonds are reported as light blue dashed lines.