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Supplementary Information

Insights into the Intrinsic Factors Affecting the NIR Reflectance Based on Rylene Diimide Molecules

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General Information

The anhydride BDA, NDA and PDA as well as other reactants (e. g. various alkyl amine) were purchased from Sigma Aldrich or Alfa Aesar and used as received. NMR was measured on Bruker 300MHz using $CDCl_3$ or D_2SO_4 as solvent. SEM images were obtained by using a JEOL/JSM-6340F instrument. XRD was measured on Bruker D8 Advance XRD. The X-ray Diffractometer used Cu Kα (λ = 1.5405 Angstrom) radiation with 2θ from 10° to 70°. FTIR were taken on a FTIR Perkin Elmer Frontier. The reflectance spectra were obtained on a UV-Vis-NIR Lambda 950 instrument. A 150 mm integrating sphere accessory was used to measure the diffuse reflectance of the samples. 300 mg powder samples were grinded with a mortar and pestle homogenously and pressed into cylinders with a diameter of 0.5 inch for the test.

The average reflectance was calculated according to the following equation:

$$R_{ave}$$= Sum of Reflectance (a nm to b nm)/Range(a-b)

Where a and b are the starting and end wavelength of the range.

The grain size was calculated according to the Scherrer Equation:

$$D = K\lambda/\beta \cos\theta$$

where K is Scherrer constant (0.94), λ is 1.54056 Å, β is the full width at half maxima of the diffraction peak, and θ is diffraction angle.

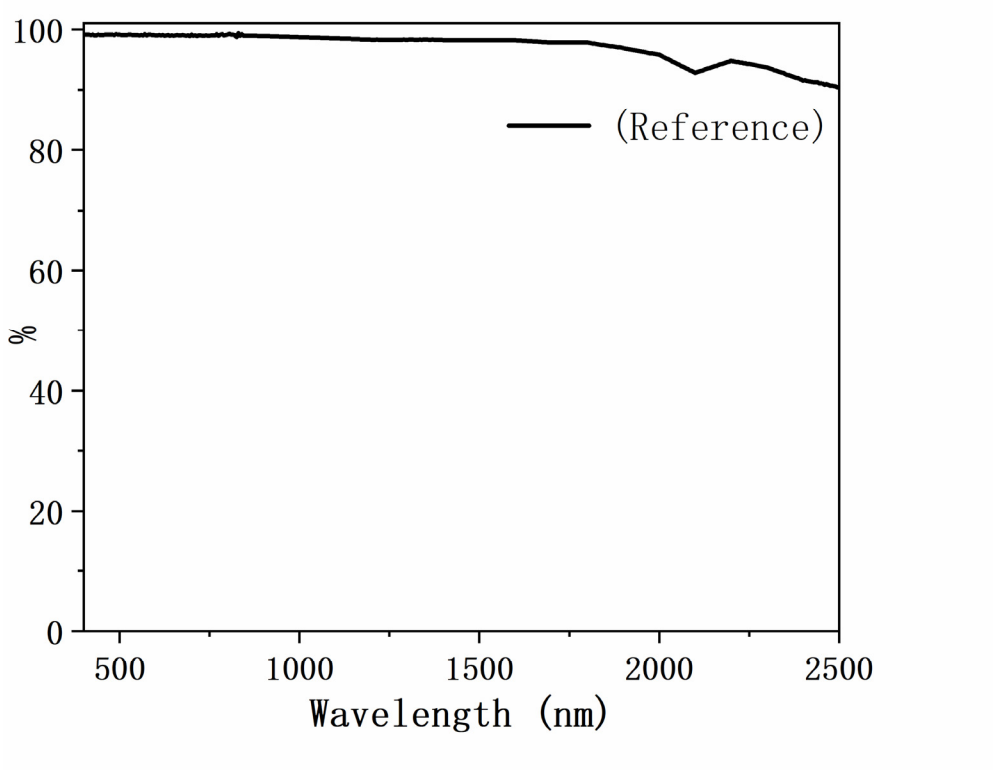
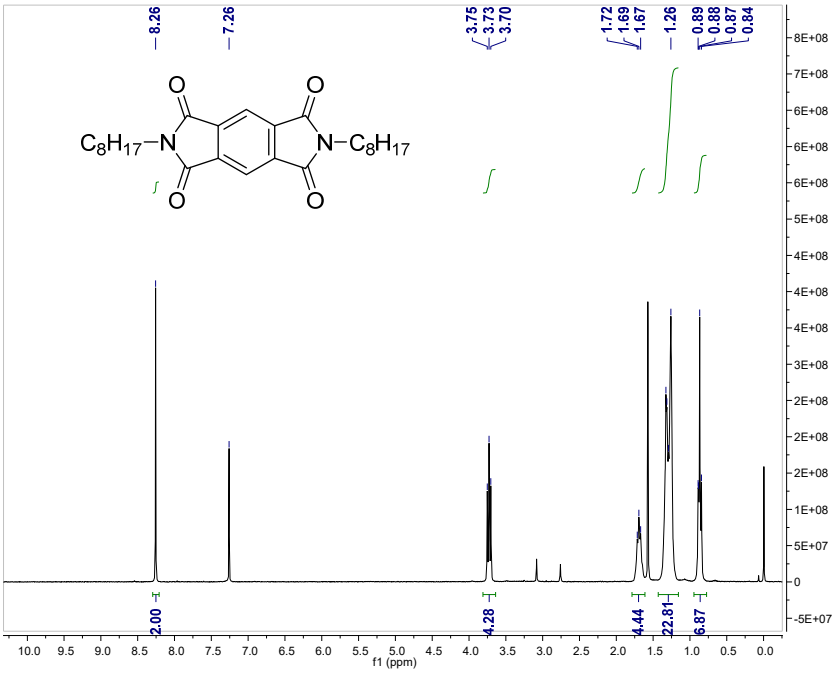


Figure S1. Reference reflectance

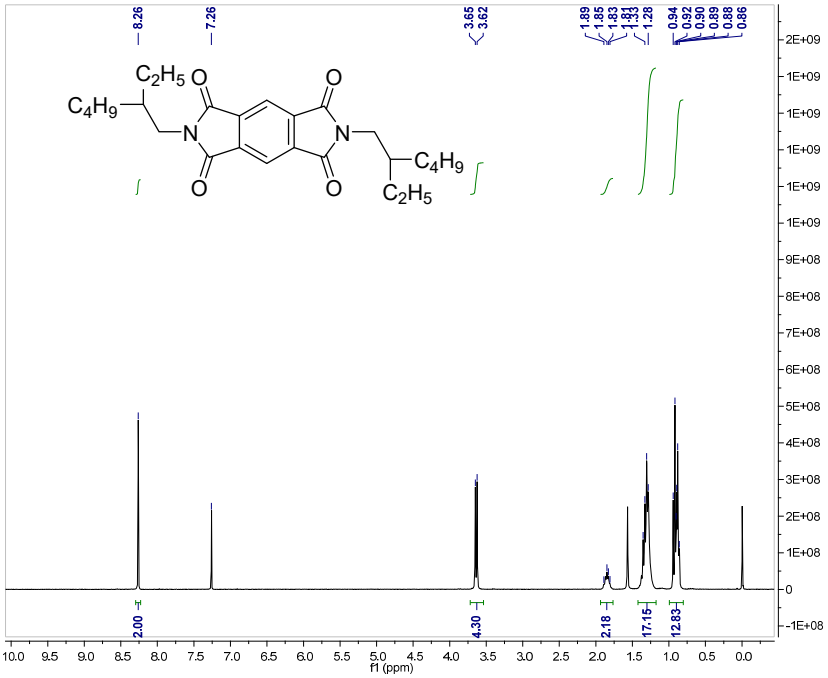
^{1}H NMR Spectra

BDI-C_8



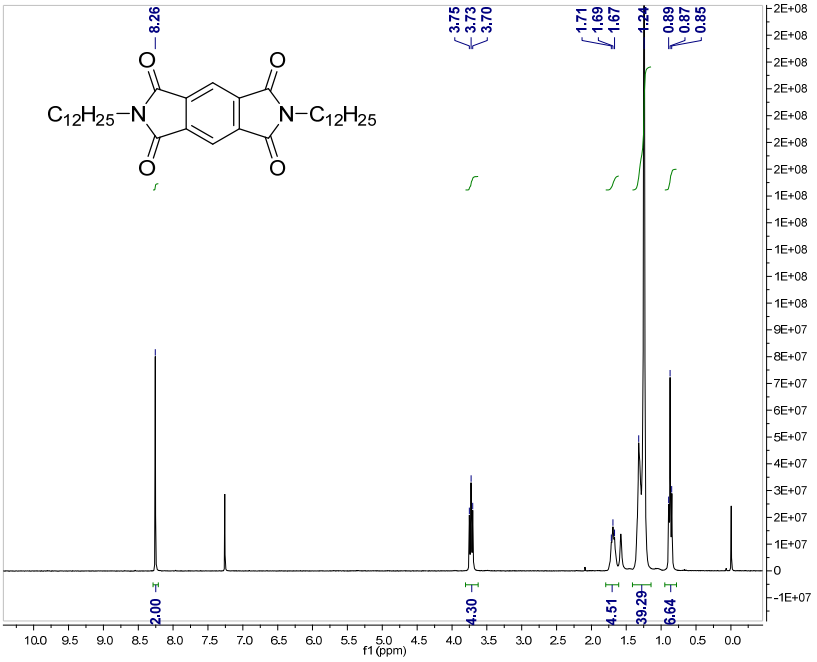
^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.26 (s, 2H), 3.73 (t, 4H), 1.72-1.67 (m, 4H), 1.32-1.26 (m, 20H), 0.89-0.84 (m, 6H)

BDI-C_2C_6



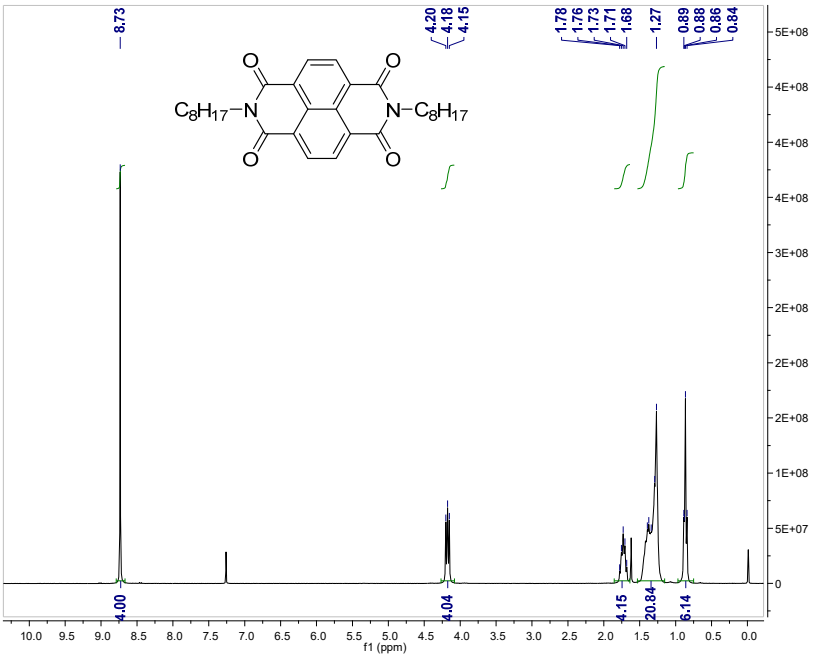
^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.26 (s, 2H), 3.33 (d, 4H), 1.81-1.89 (m, 2H), 1.35-1.28 (m, 16H), 0.94-0.86 (m, 12H)

BDI-C_{12}



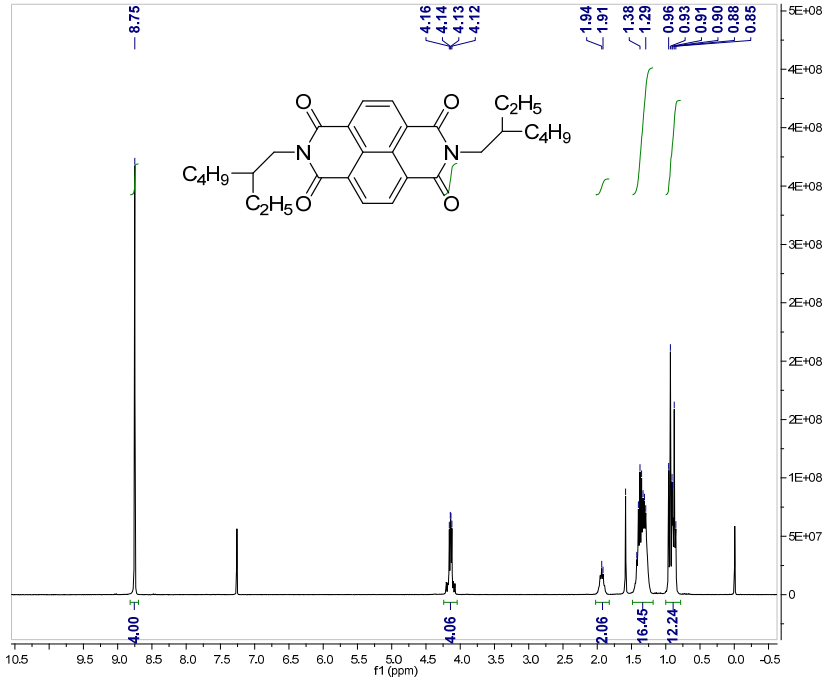
^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.26 (s, 2H), 3.73 (d, 4H), 1.71-1.67 (m, 4H), 1.32-1.24 (m, 36H), 0.89-0.85 (m, 6H)

NDI-C_8



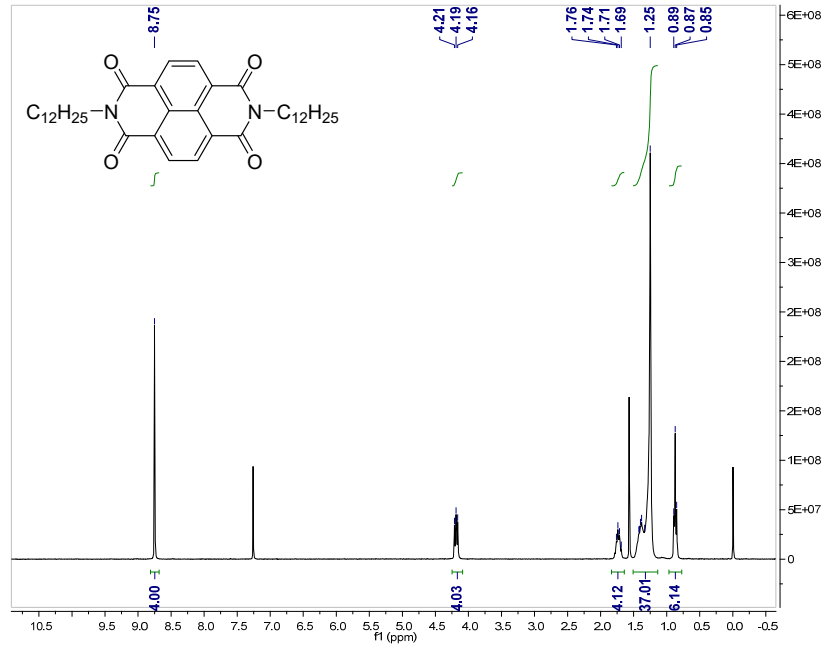
^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.73 (s, 4H), 4.18 (t, 4H), 1.78-1.68 (m, 4H), 1.39-1.27 (m, 20H), 0.89-0.84 (m, 6H)

NDI-C_2C_6



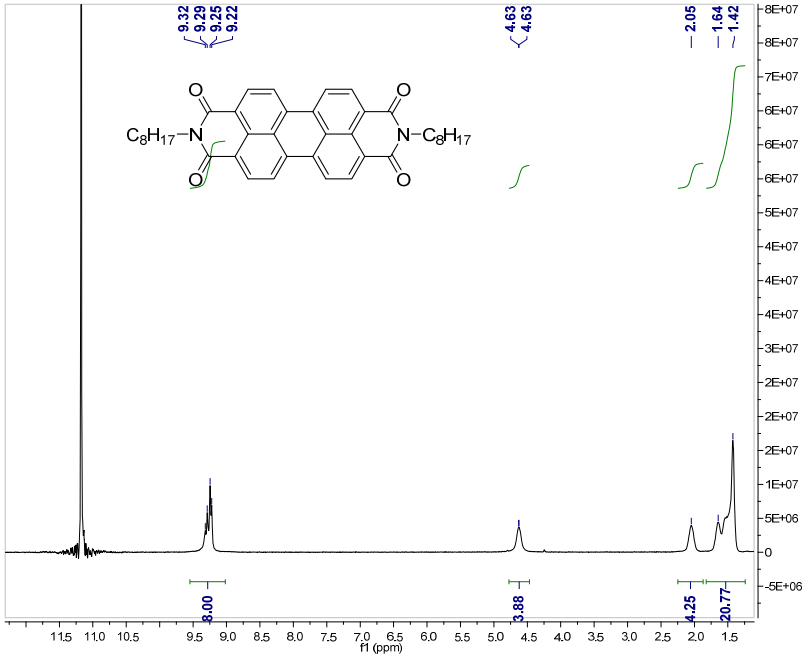
^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.75 (s, 4H), 4.16-4.12 (d, 2H), 1.89-1.98 (m, 2H), 1.40-1.29 (m, 16H), 0.96-0.85 (m, 12H)

NDI-C_{12}



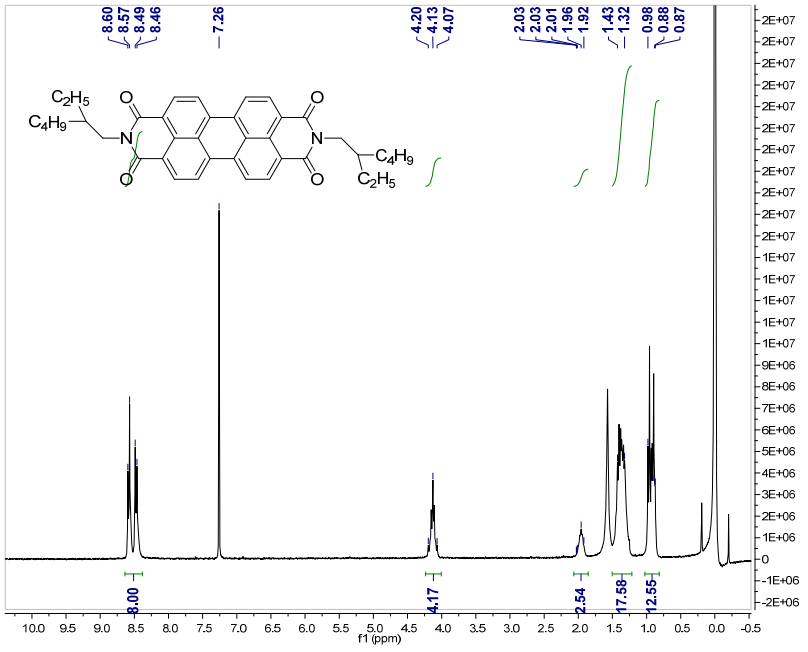
^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.75 (s, 4H), 4.19 (t, 4H), 1.76-1.69 (m, 4H), 1.42-1.25 (m, 36H), 0.89-0.85 (m, 6H)

PDI-C8



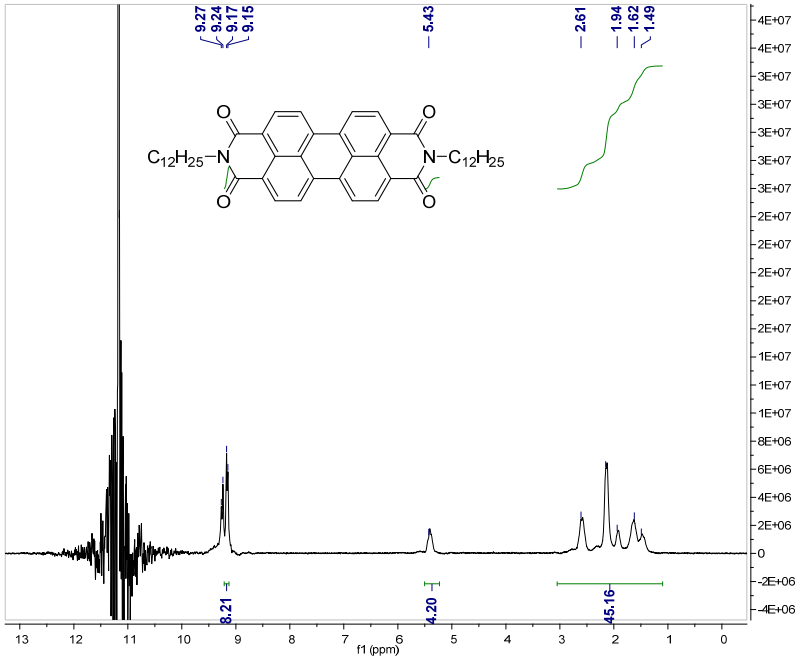
^{1}H NMR (300 MHz, D_2SO_4): δ = 9.32-9.22 (m, 8H), 4.63 (s, 4H), 2.05 (s, 4H), 1.64-1.42 (m, 20H), 0.89-0.84 (m, 6H)

PDI-C2C6



^{1}H NMR (300 MHz, $CDCl_3$): δ =δ = 8.60-8.46 (m, 8H), 4.20-4.07 (d, 2H), 2.03-1.92 (m, 2H), 1.43-1.32 (m, 16H), 0.98-0.87 (m, 12H)

PDI-C_{12}



^{1}H NMR (300 MHz, D_2SO_4): δ = 9.27-9.15 (m, 8H), 5.43 (s, 4H), 2.61-1.49 (m, 46H)