

Synthesis and very large mechano- and thermo-hypsochromic luminescence of a new-type DPP-based derivative

Zhongwei Liu, Kai Zhang, Qikun Sun, Zhenzhen Zhang, Liangliang Tang, Shanfeng Xue, Dongmei Chen, Haichang Zhang,* and Wenjun Yang*

Key Laboratory of Rubber-plastics of Ministry of Education/Shandong Province (QUST), School of Polymer Science & Engineering, Qingdao University of Science & Technology, 53-Zhengzhou Road, Qingdao, 266042, P. R. China. *E-mail: haichangzhang@hotmail.com, ywjph2004@qust.edu.cn

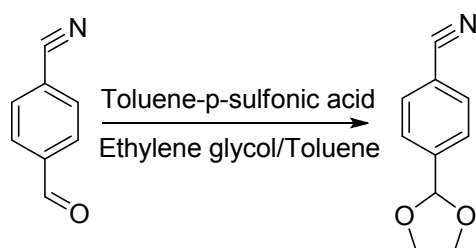
CONTENTS

S1. Synthesis

S2. Supporting Figures

S3. Supporting Tables

Synthesis of S1 (4-(1,3-dioxolan-2-yl)benzonitrile)



To a solution of 4-cyanobenzaldehyde (15.0 g, 114.4 mmol) in toluene (300 mL) was added ethylene glycol (11.5 mL, 206 mmol) followed by pyridinium-*p*-toluene-sulfonic acid (1.5 g, 8.7 mmol) and then heated at 130 °C in Dean-Stark apparatus with continuous exclusion of water. After the formation of H₂O cease. Cooled the reaction solution to room temperature. The solution was washed with saturated aqueous NaHCO₃ (100 mL) and brine (50 mL × 3). The organic layer was dried over anhydrous MgSO₄, and then concentrated via rotary evaporation. The raw product was purified by column chromatography (silica gel; petroleum/ethyl acetate, 1/4, v/v)

to get 4-(1,3-dioxolan-2-yl)benzotrile as an off white solid. (Yield: 18.53 g, 92%).

^1H NMR (500 MHz, Chloroform-d) δ 7.62 (ddt, $J = 41.5, 7.4, 3.0$ Hz, 4H), 5.89-5.77 (m, 1H), 4.15-3.98 (m, 4H).

S2. Supporting Figure

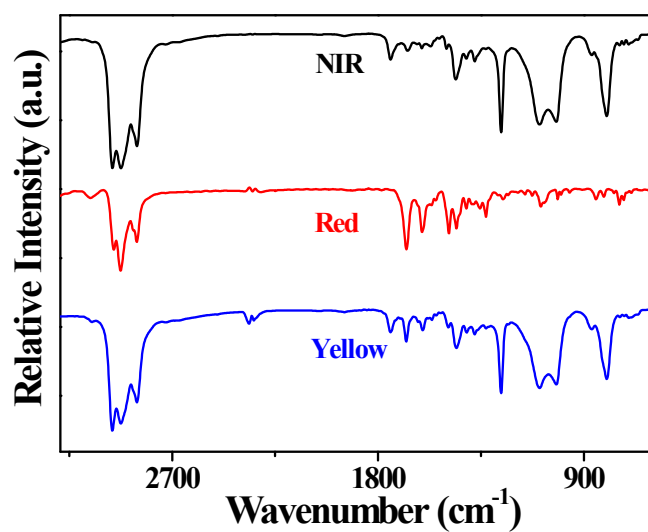
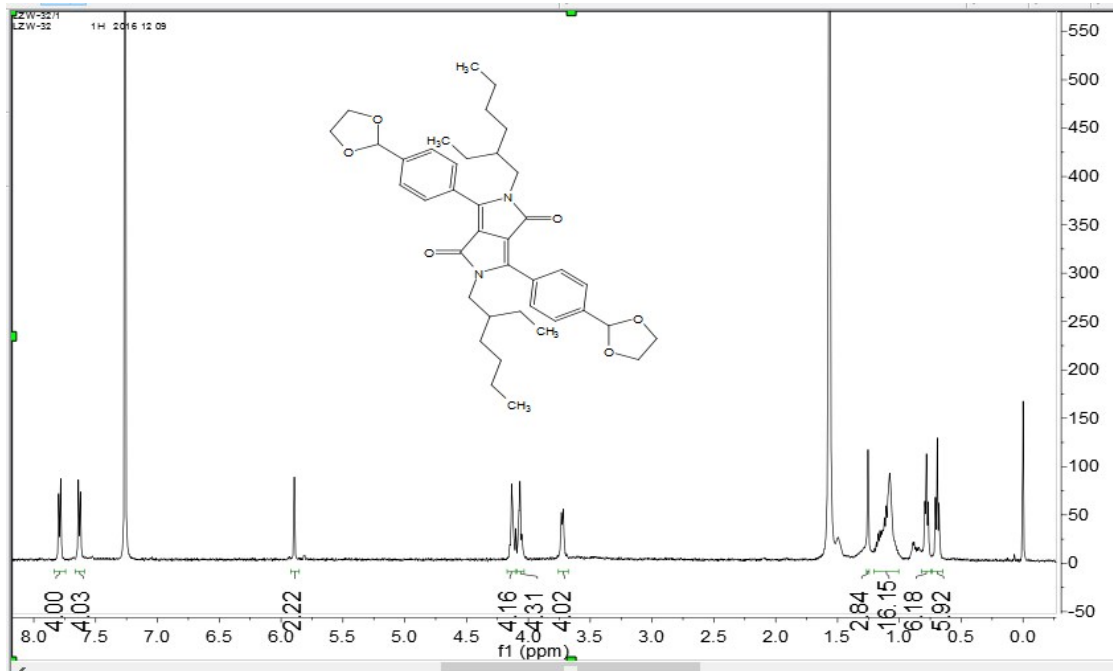
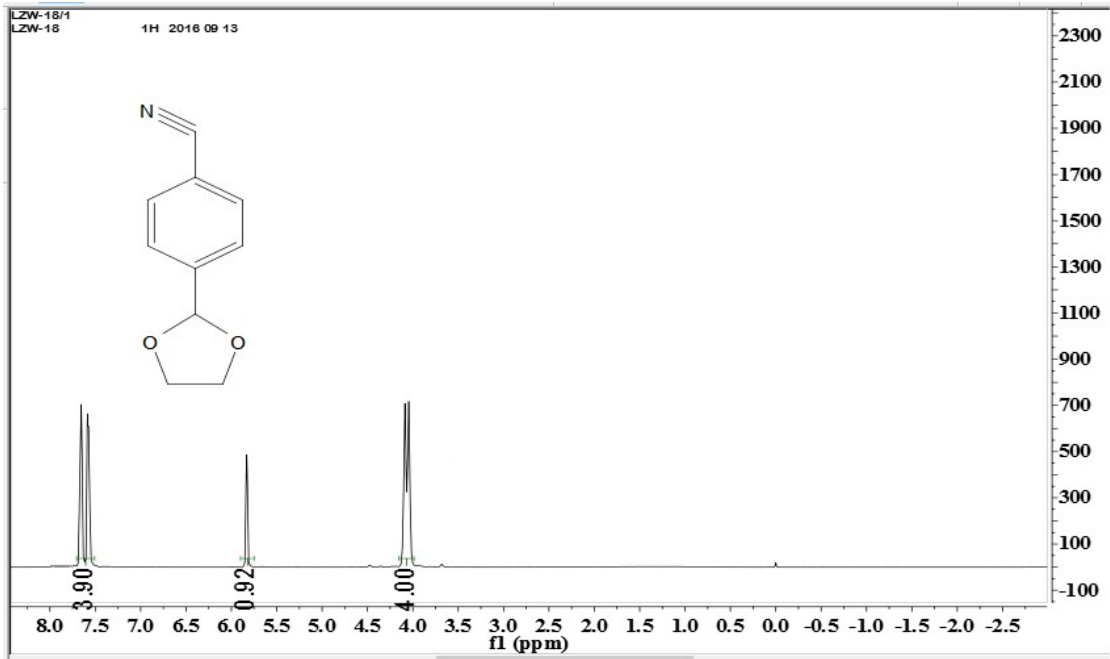
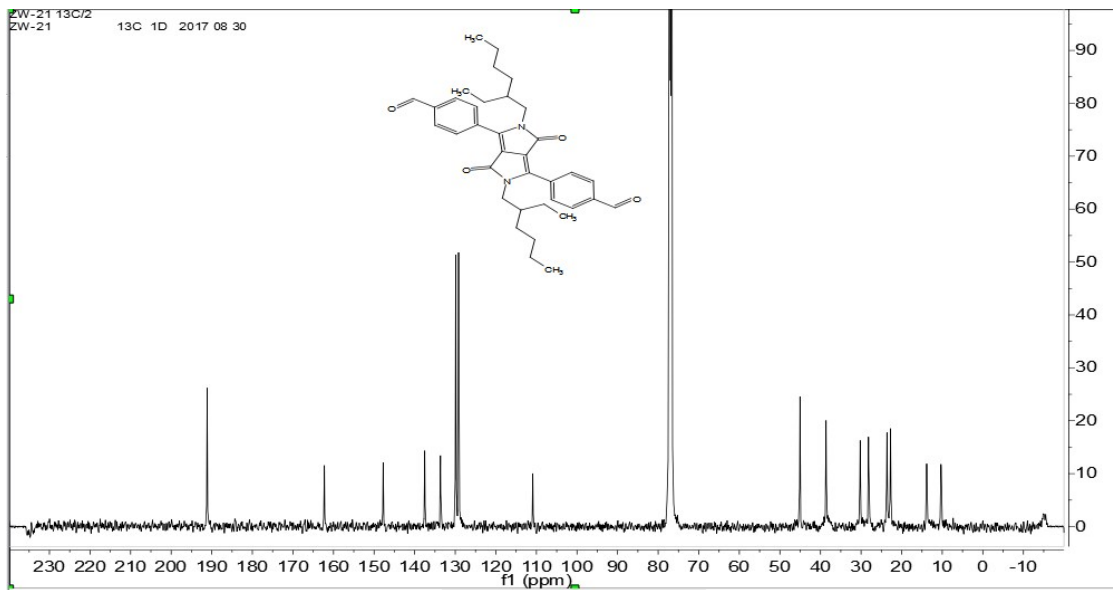
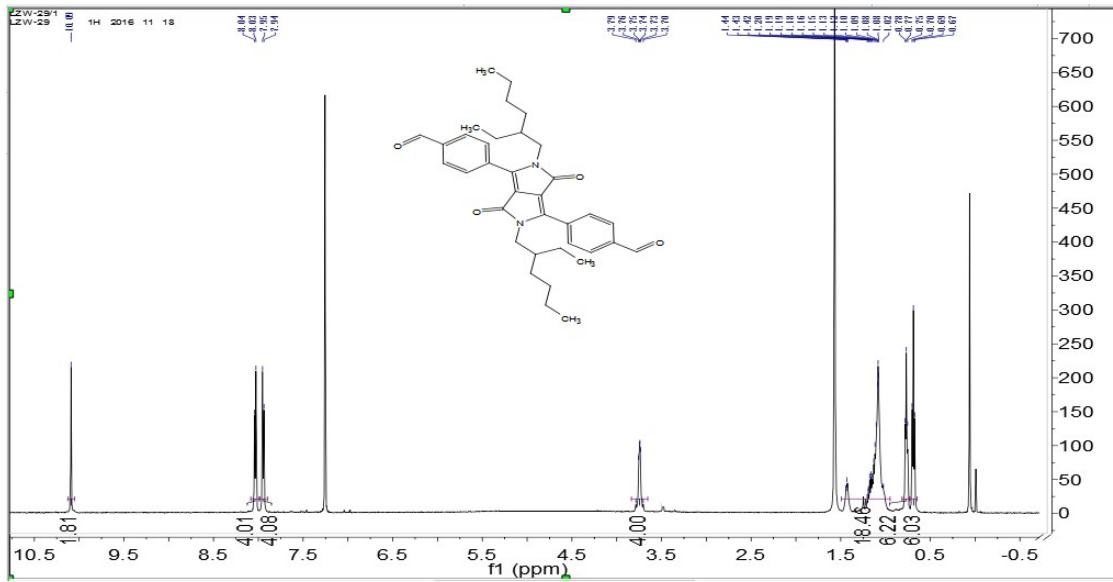
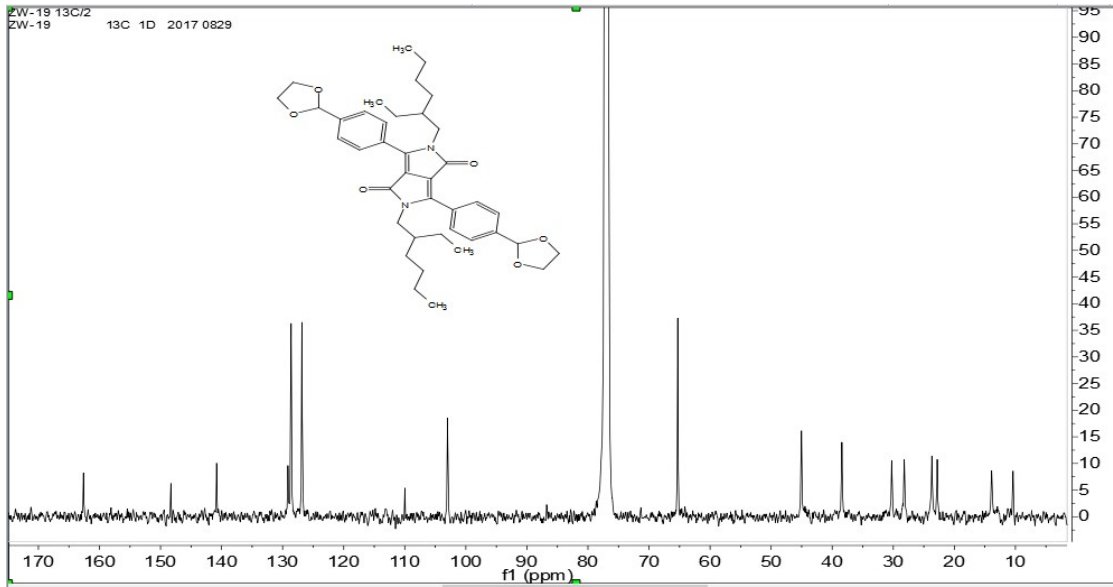
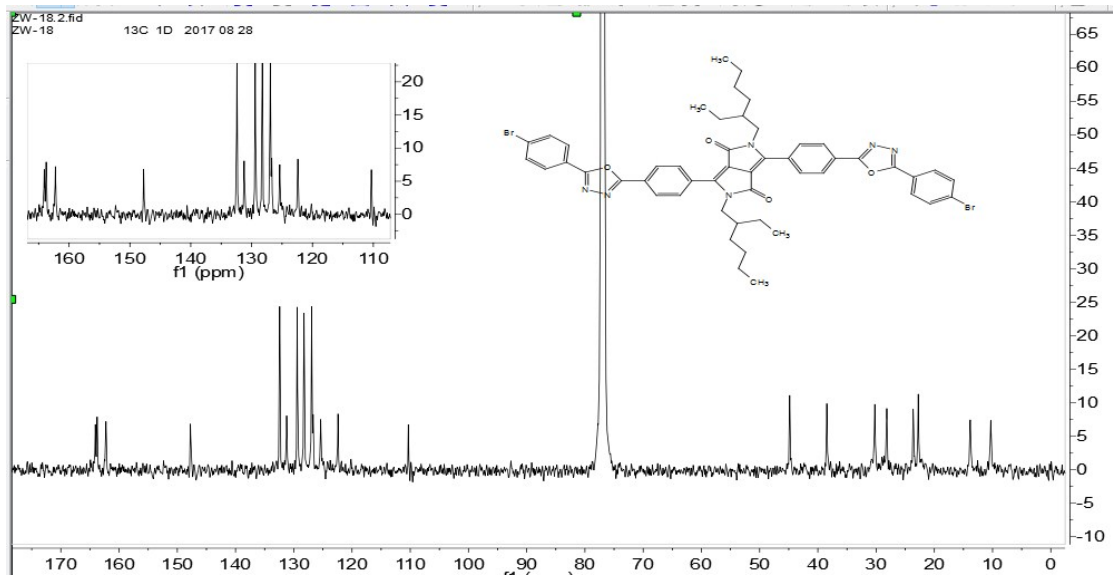
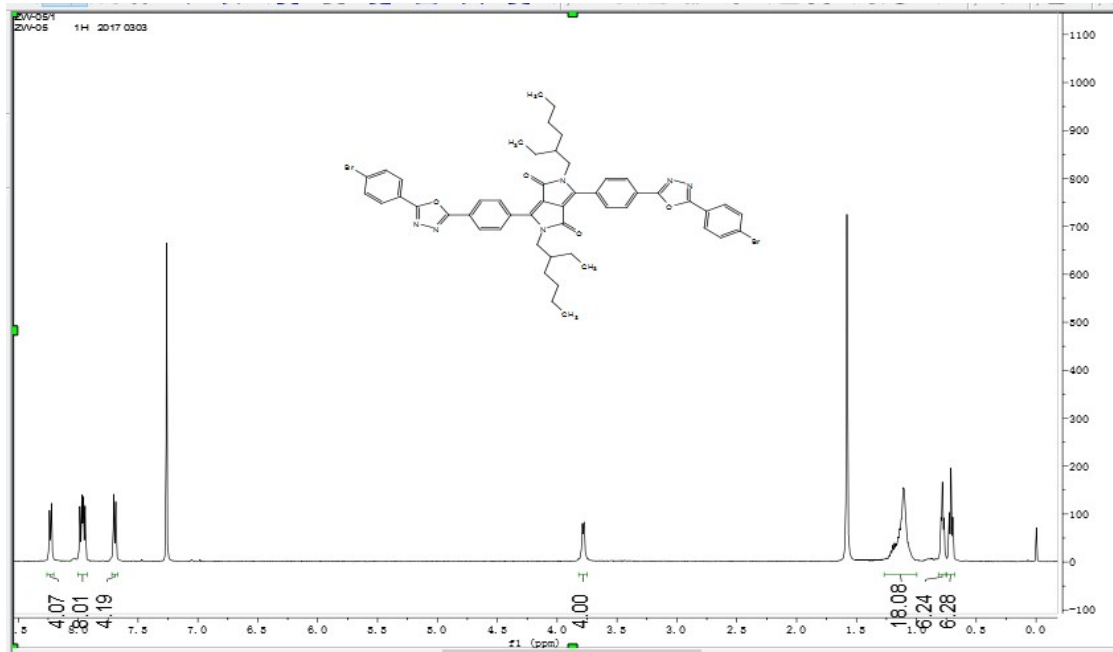


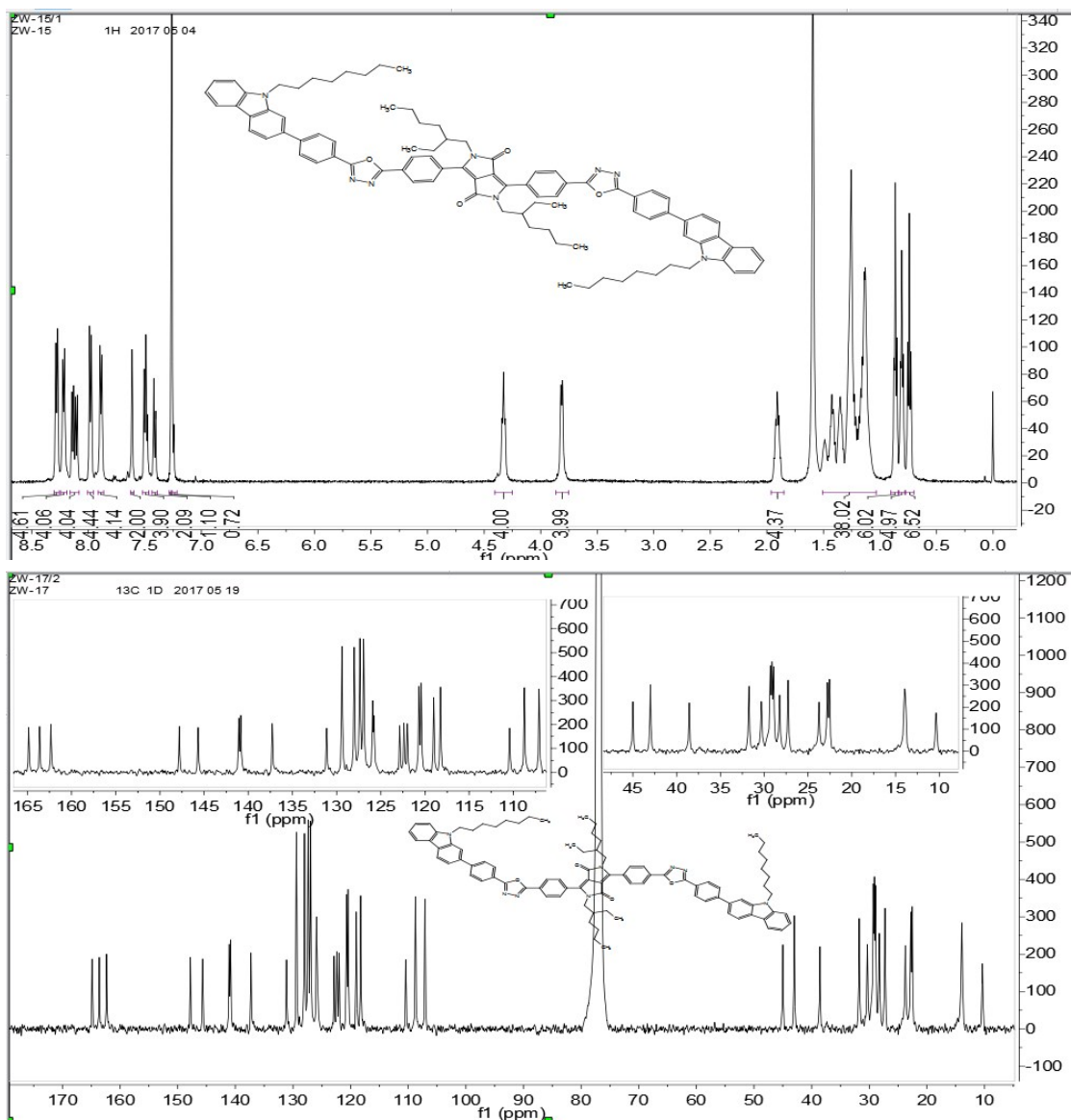
Figure S1. FTIR spectra of CODPP solids with different emission colors.

^1H NMR and ^{13}C spectra of the compounds as follows









SI-3. Supporting Tables

Table S1 The solution fluorescence quantum yields (%) and the molar extinction coefficients ($M^{-1} cm^{-1}$) of CODPP in different solvents.

Solvents	PhMe	CHCl ₃	THF	DMF
Fluorescence quantum yield (%)	74.8	75.1	72.3	67.0
The molar extinction coefficients	54000	50300	59000	52700

Table S2 The solid fluorescence quantum yields (%) of CODPP in different states.

States	Pristine	Ground	Annealed
CODPP	15%	46%	95%

