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Tuning Solid-State Fluorescence of Chalcone Crystals Via Molecular Coplanarity and J-Aggregates Formation

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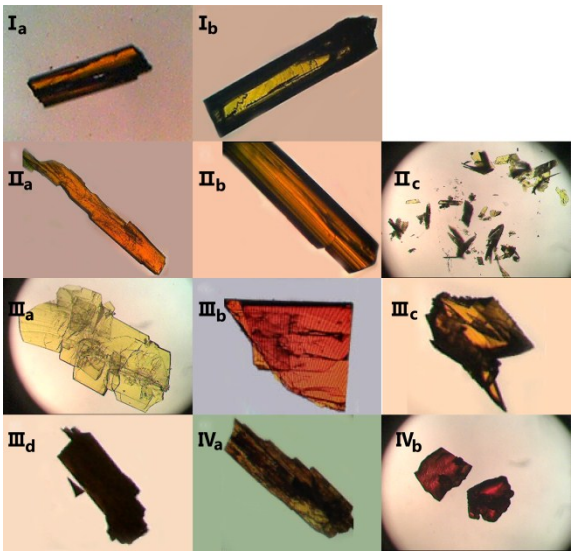

Fig. 1S Microscopy graphs of all forms.

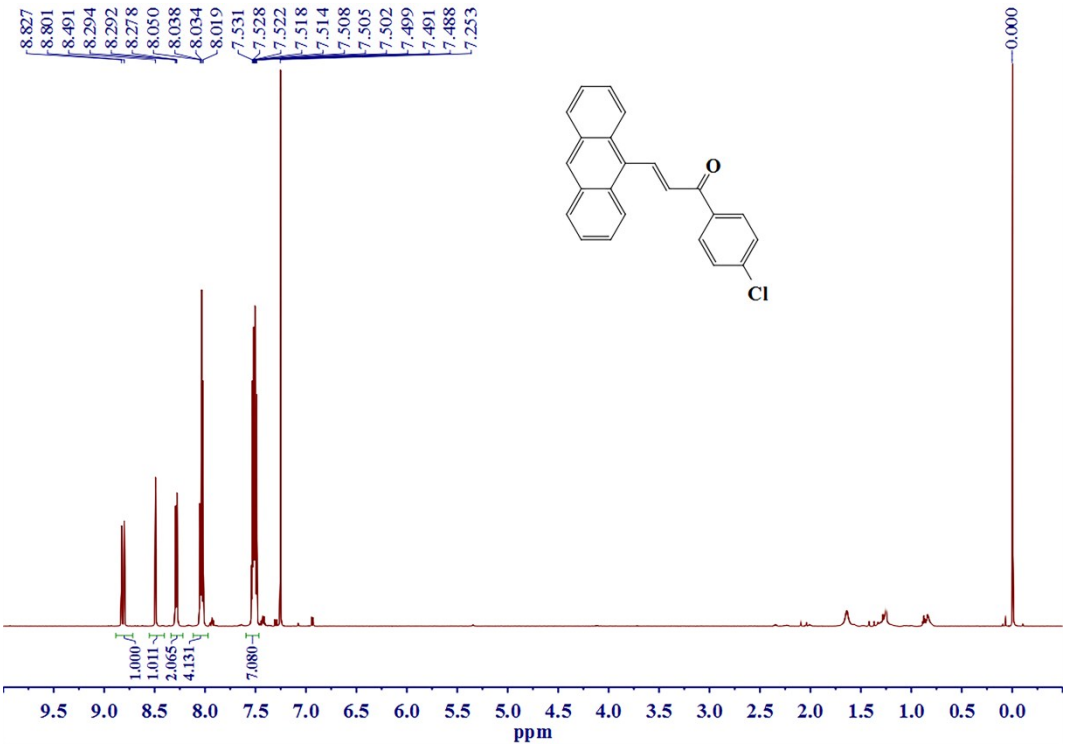

Fig. 2S ^{1}H NMR spectrum of ACPPO.

Assignments of each H in the NMR spectrum: δ (ppm) 8.81 (Ar-H from anthracene ring, 1H), 8.49 (H of CH from 1-ethylene, 1H), 8.36-8.19 (Ar-H from benzene ring, 2H), 8.04 (Ar-H from anthracene ring, 4H), 7.63-7.46 (the rest Ar-H from anthracene and benzene ring and another H of 1-ethylene, 7H).

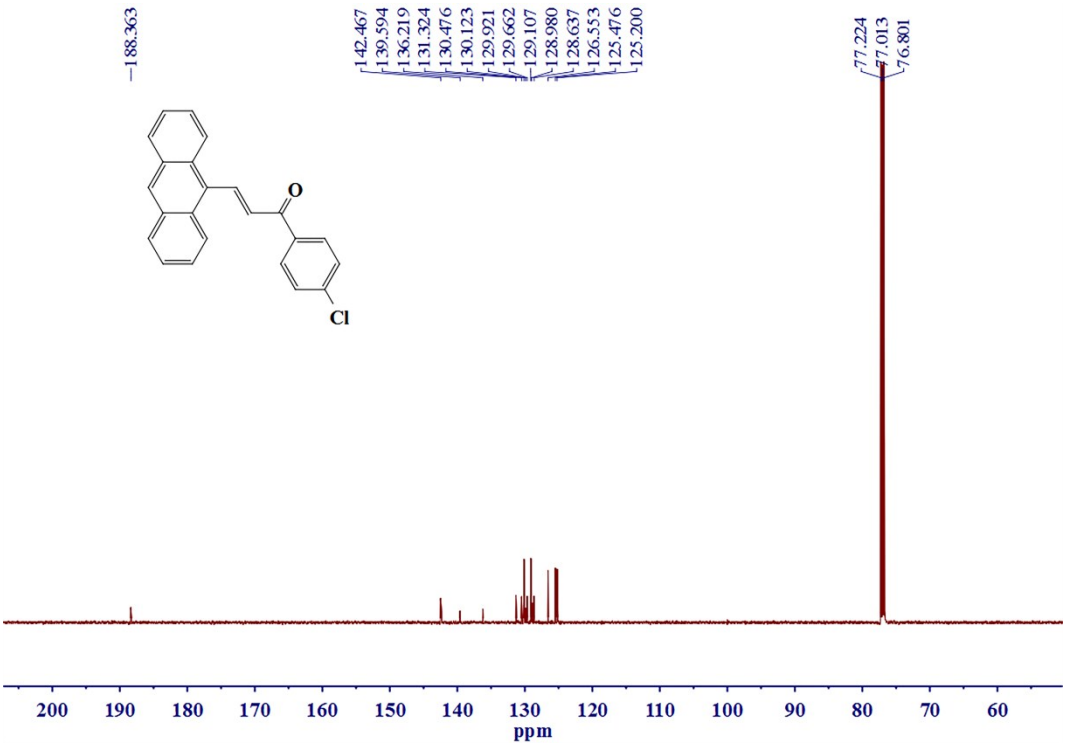

Fig. 3S ^{13}C NMR spectrum of ACPPO.

Assignments of C in the NMR spectrum: δ (ppm) 188.36 (C=O), 142.47 (C*= C-CO), 139.59 ((Ph)C-Cl), 136.22 (O=C-C*(Ph)), 131.32-125.48 (the rest Ar-C from pyrene and benzene rings), 125.20(C=C*-CO)

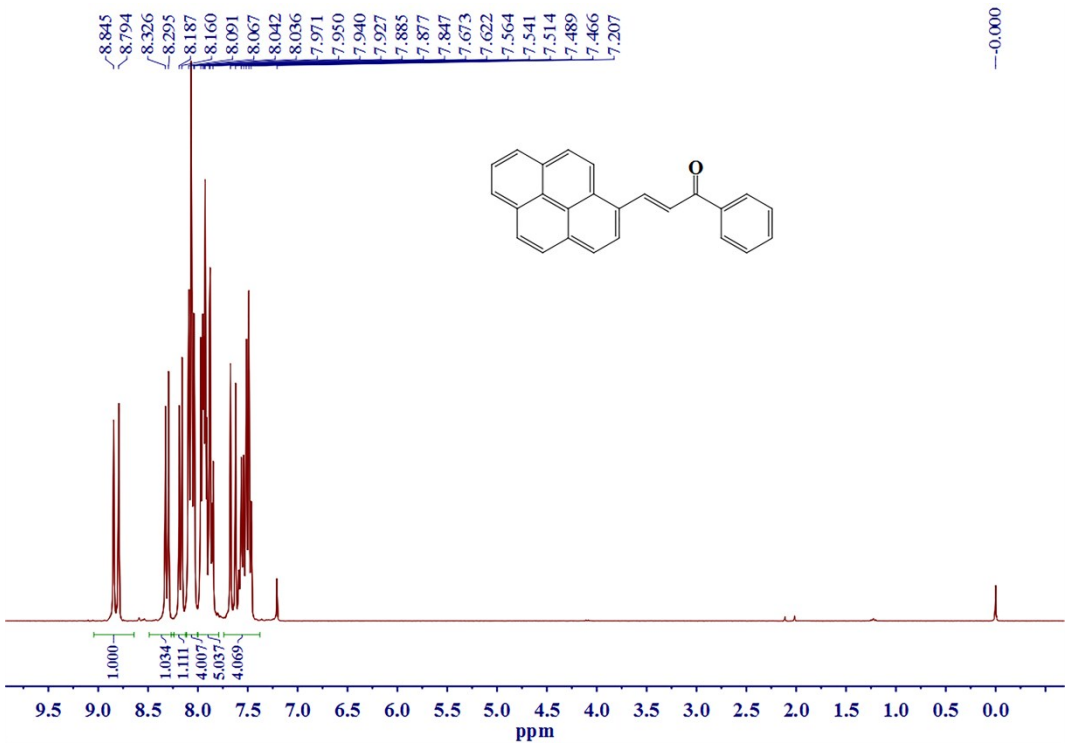

Fig. 4S ^{1}H NMR spectrum of PPPO.

Assignments of each H in the NMR spectrum: δ(ppm) 8.82 (Ar-H from pyrene ring, 1H), 8.31 (H of CH from 1-ethylene, 1H), 8.17 (Ar-H from pyrene ring, 1H), 8.06 (Ar-H from pyrene ring, 4H), 8.00-7.80 (Ar-H from pyrene and benzene rings, 5H), 7.65(H of CH from 1-ethylene, 1H), 7.61-7.42 (Ar-H from benzene ring).

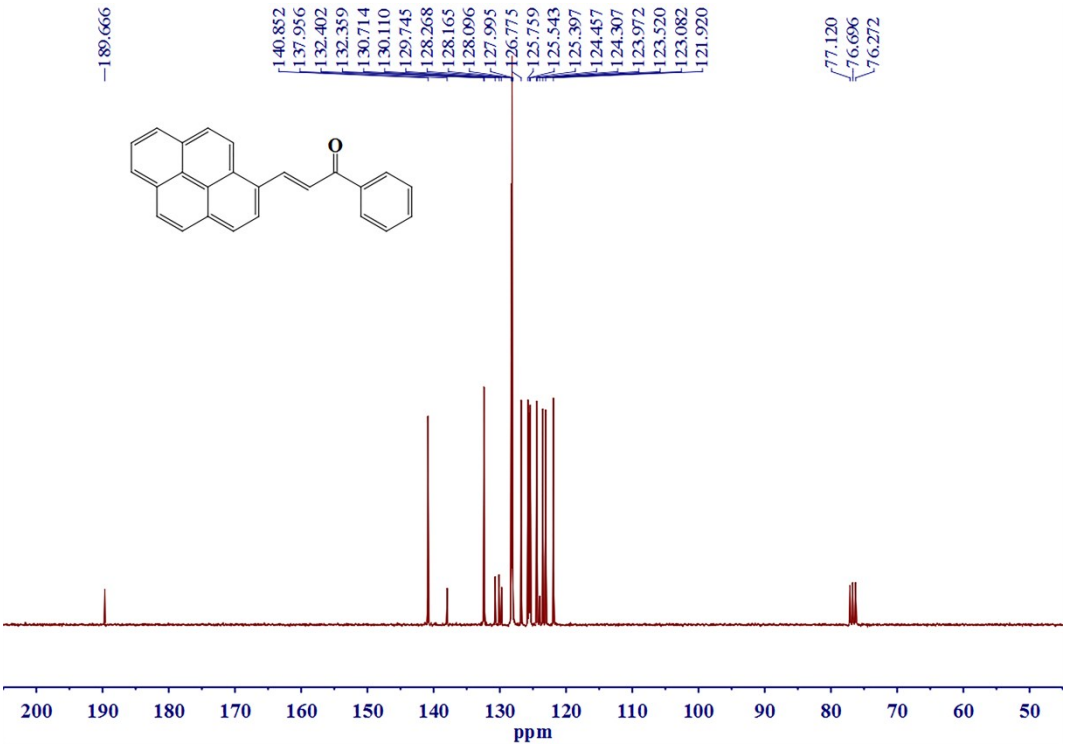

Fig. 5S ^{13}C NMR spectrum of PPPO.

Assignments of C in the NMR spectrum: δ (ppm) 189.67 (C=O), 140.85 (C*= C-CO), 137.96(O=C-C*(Ph)), 132.40-123.97, 123.08, 121.92(the rest Ar-C from pyrene and benzene rings), 123.52(C*=C-CO)

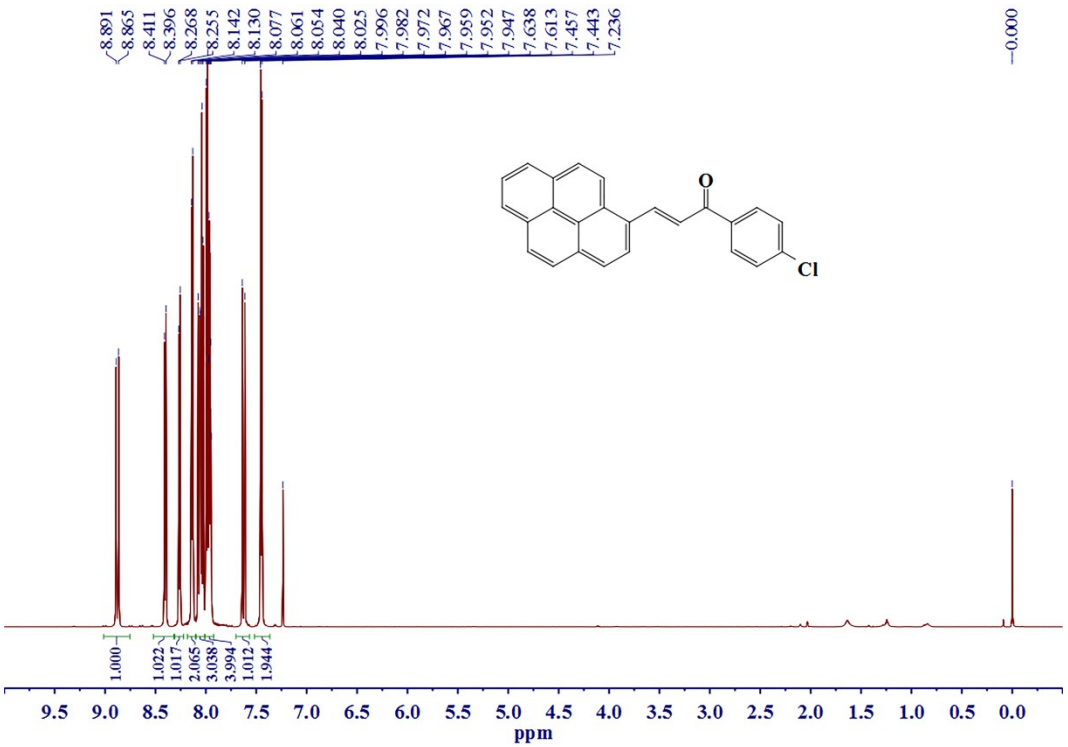

Fig. 6S ^{1}H NMR spectrum of PCPPO.

Assignments of each H in the NMR spectrum: δ(ppm) 8.88 (Ar-H from pyrene ring, 1H), 8.40 (H of CH from 1-ethylene, 1H), 8.26

(Ar-H from pyrene ring, 1H), 8.14 (Ar-H from benzene ring, 2H), 8.09-7.93 (the rest Ar-H from pyrene ring, 7H), 7.63 (another H of CH from 1-ethylene, 1H), 7.45 (the rest Ar-H from benzene ring, 2H).

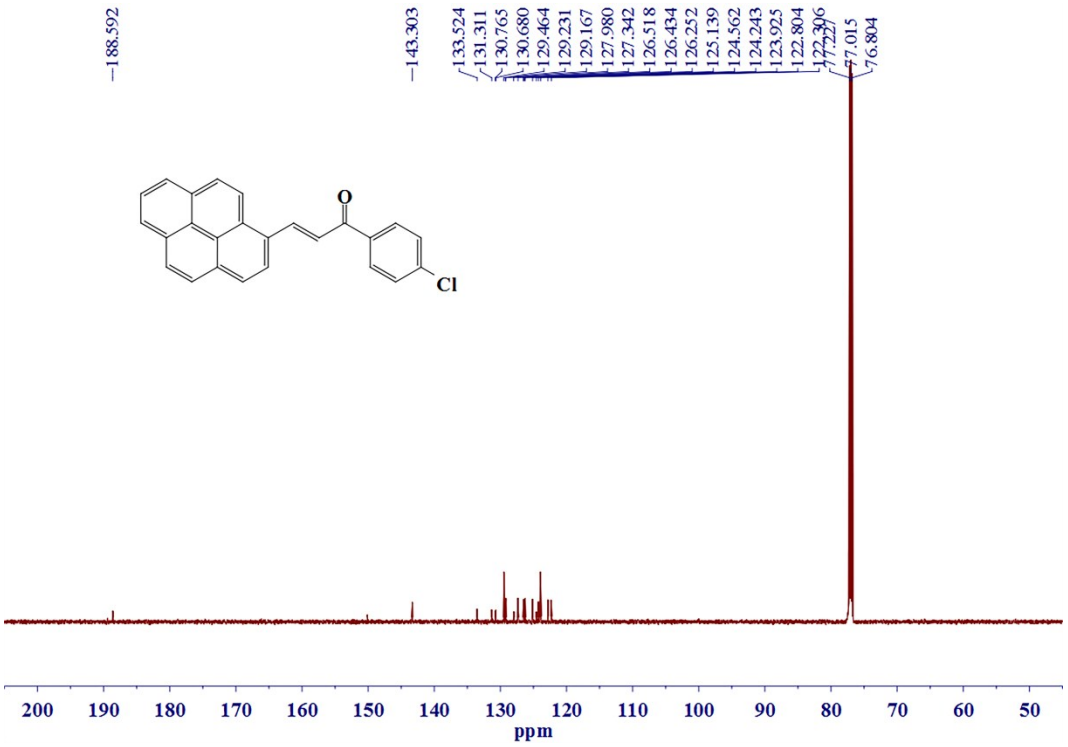

Fig. 7S ^{13}C NMR spectrum of PCPPO.

Assignments of C in the NMR spectrum: δ (ppm) 188.63 (C=O), 141.72(C*= C-CO), 139.17 ((Ph)C-Cl), 136.60 (O=C-C*(Ph)), 132.98-124.44, 122.95, 122.33 (the rest Ar-C from pyrene and benzene rings), 124.00 (C=C*-CO)

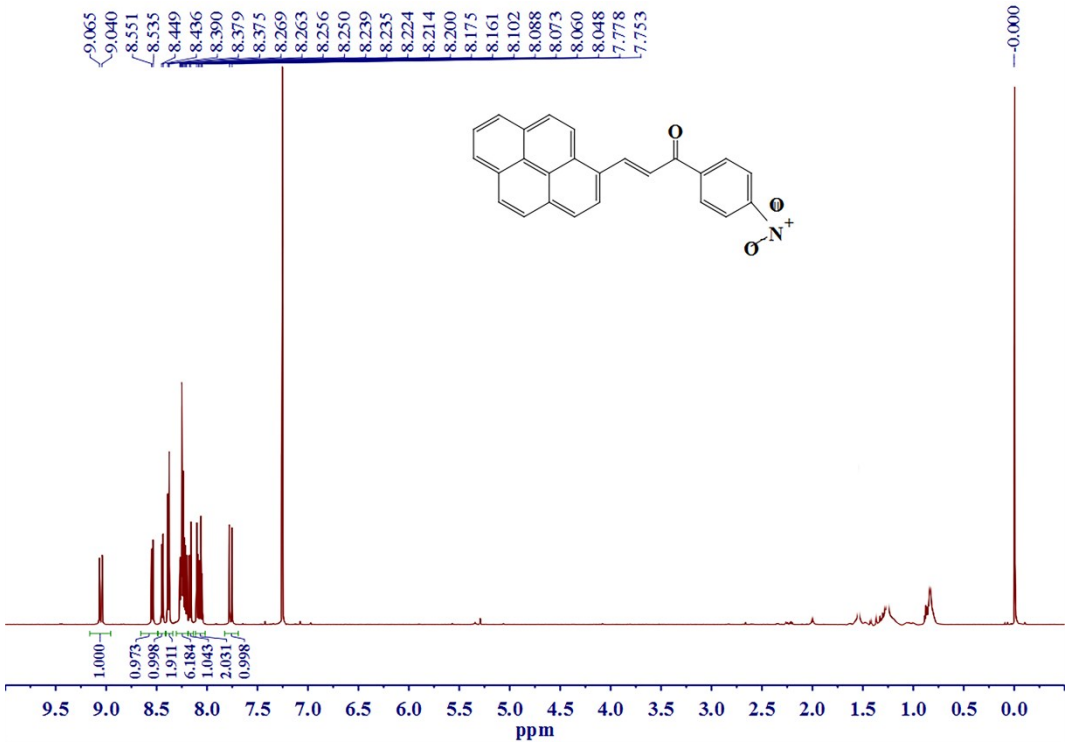

Fig. 8S ^{1}H NMR spectrum of PNPPO.

Assignments of each H in the NMR spectrum: δ(ppm) 9.05 (Ar-H from benzene ring, 1H), 8.54 (Ar-H from pyrene ring, 1H), 8.44-8.33 (Ar-H from benzene ring, 1H), 8.33-8.19 (Ar-H from pyene ring, 6H), 8.14-8.01 (Ar-H from pyene ring, 2H), 8.17 (H of CH from 1-ethylene, 1H), 7.77 (another H of CH from 1-ethylene, 1H).

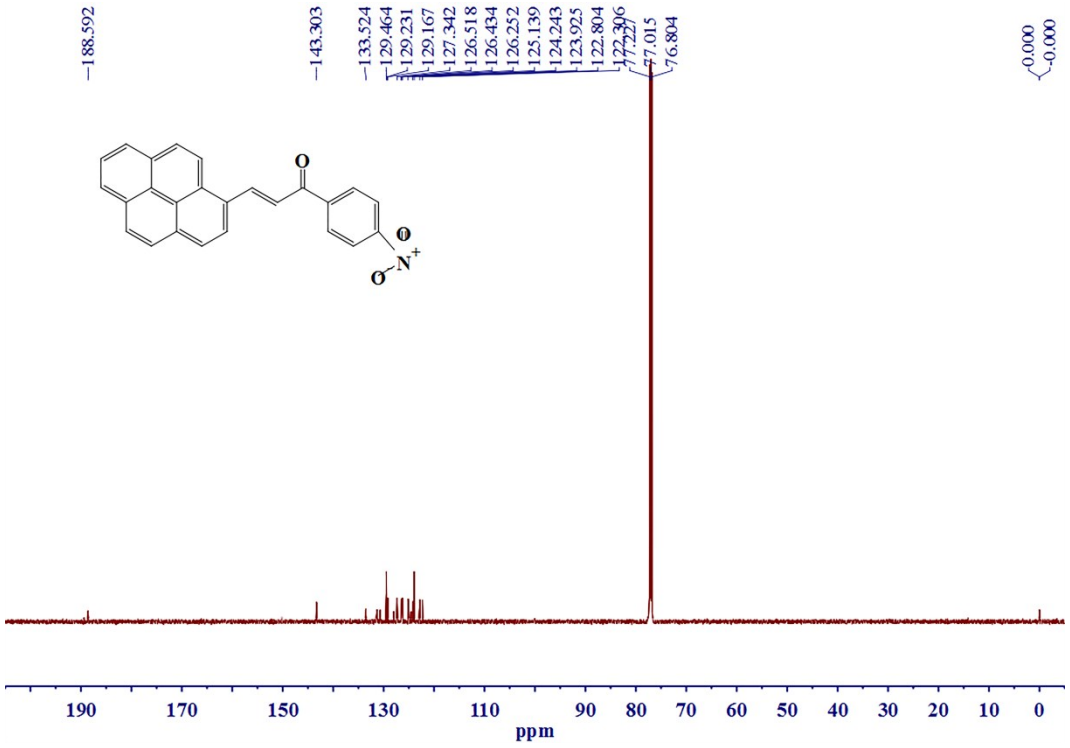

Fig. 9S ^{13}C NMR spectrum of PNPPO.

Assignments of C in the NMR spectrum: δ (ppm) 188.59 (C=O), 143.30 ((Ph)C-NO_2), 133.52 (O=C-C*(Ph)), 131.31 (C*= C-CO), 130.77-124.24, 122.80, 122.31 (the rest Ar-C from pyrene and benzene rings), 123.92(C= C*-CO)

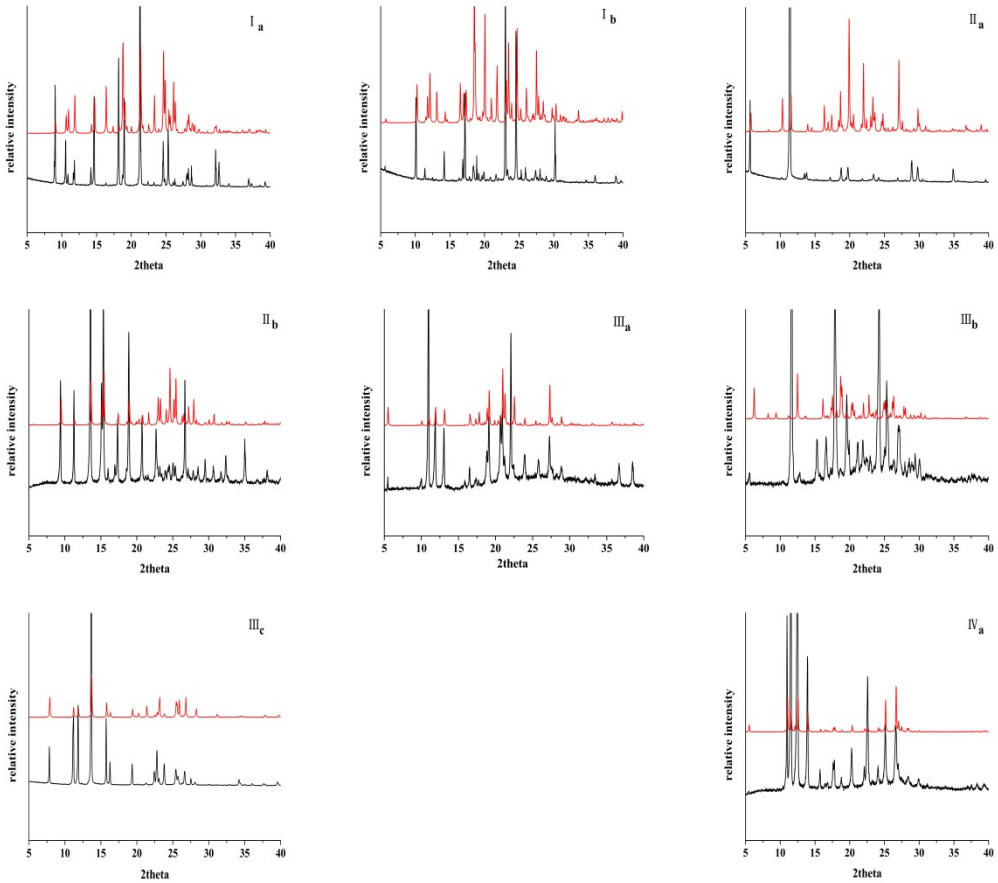

Fig. 10S Comparing of PXRD experimental patterns (black) of crystals with simulated patterns (red).

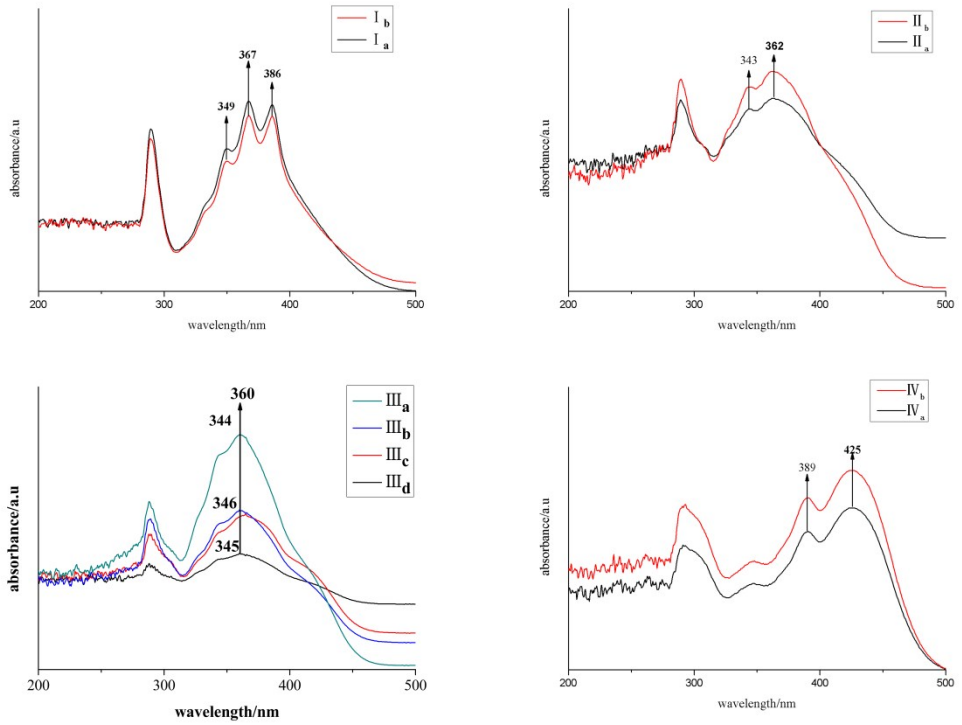

Fig. 11S Absorption spectra of crystals in acetonitrile solvent.

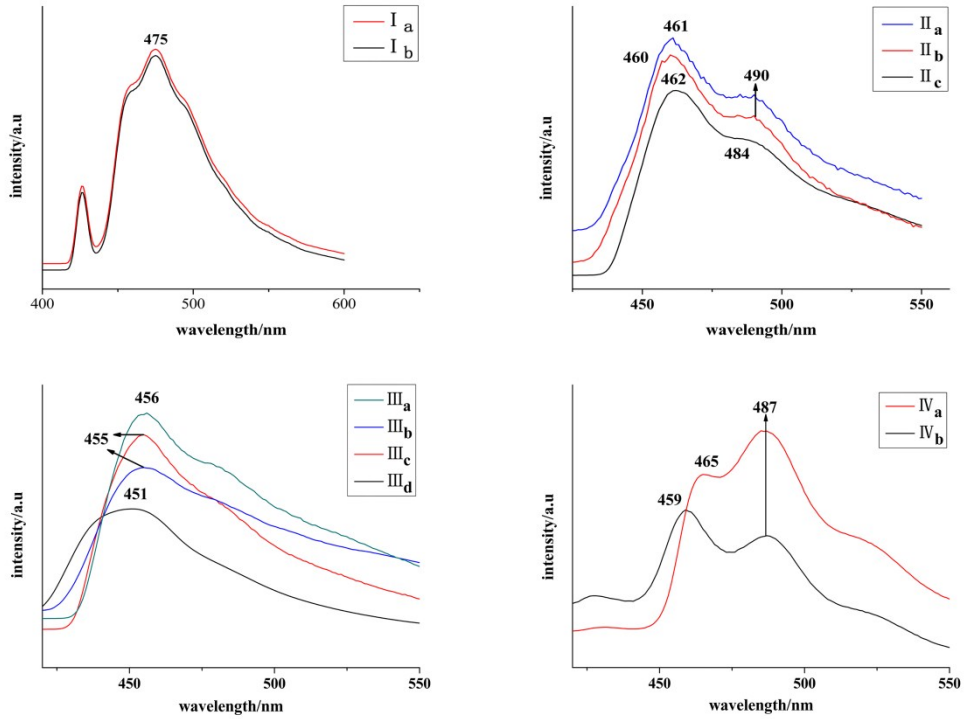

Fig. 12S Fluorescence spectra (λ_{ex} = 365 nm) in cyclohexane solution for all forms.

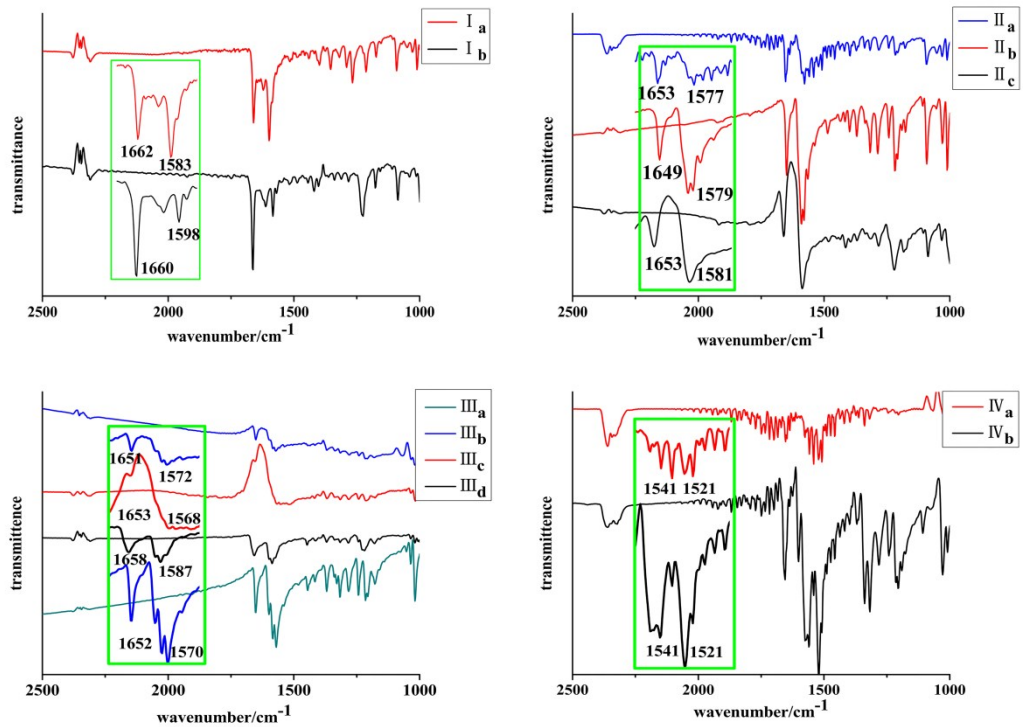

Fig. 13S IR spectra of crystals.

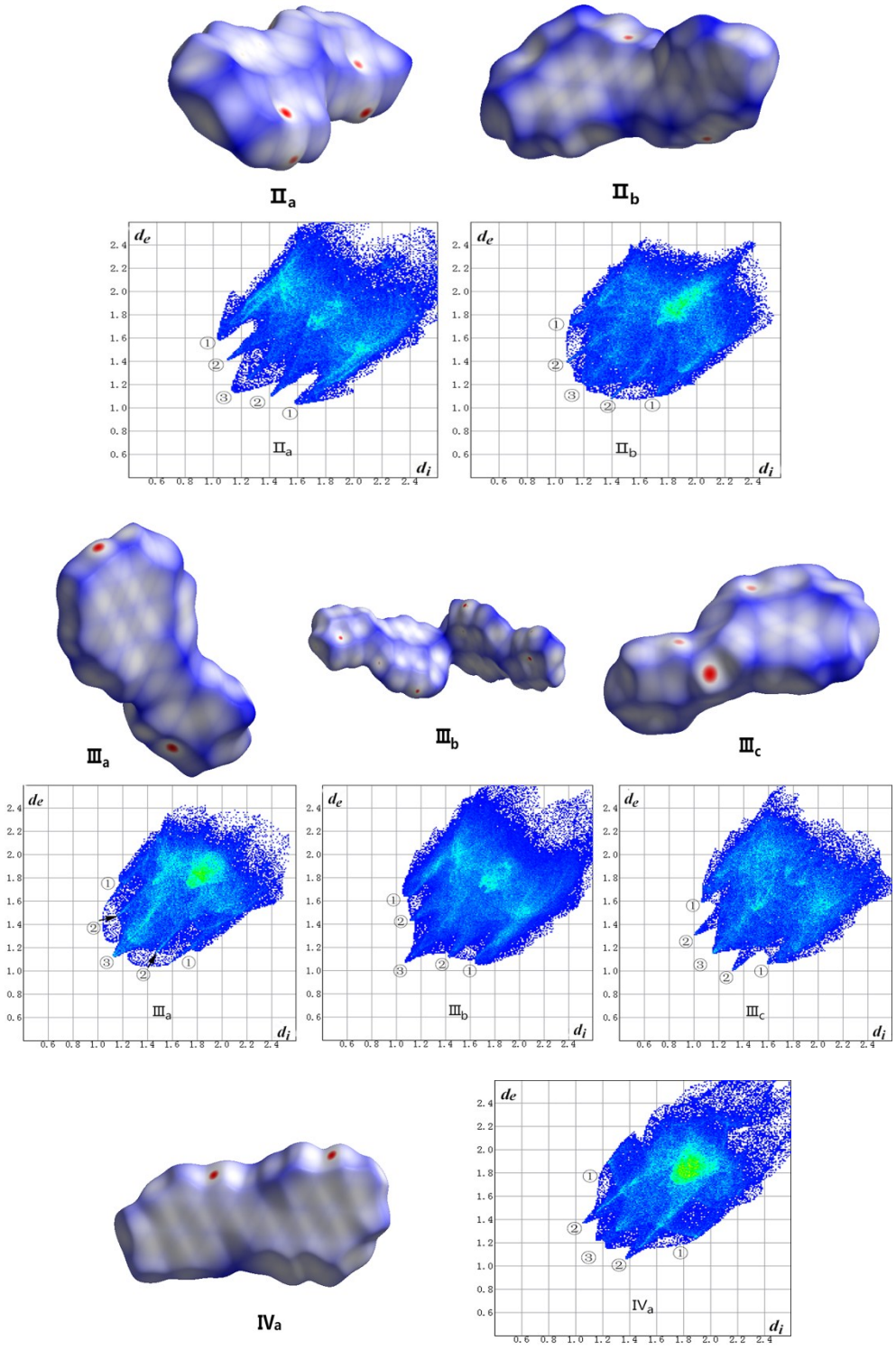

Fig. 14S Hirshfeld surface mapped with d_{norm} and Fingerprint plots of crystals

Table. 1S Solvents for crystal preparation.

Chalcone	**I**		**II**		
Form	**I_a**	**I_b**	**II_a**	**II_b**	**II_c**
Solvent[a]	Acetic acid/ ethyl acetate	Ethanol	Acetic acid/ ethyl acetate	Ethyl acetate / dichloromethane	Isopropanol

Chalcone	**III**				**IV**	
Form	**III_a**	**III_b**	**III_c**	**III_d**	**IV_a**	**IV_b**
Solvent[a]	Ethanol/ ethyl acetate	Ethanol/ ethyl acetate	Actonitrile/ chloroform	Isopropanol	Acetonitrile /dichloromethane	Acetonitrile /dichloromethane

[a] The volume ratio of mixed solvents above was v:v = 1:1.

Table. 2S Melting point, enthalpy and decomposition temperature range of all crystals

Chalcone	**I**		**II**		
Form	**I_a**	**I_b**	**II_a**	**II_b**	**II_c**
Melting point/°C	137	144	144,156	162	118,131
Enthalpy/J·g^{-1}	71.49	108.88	61.18	76.12	33.62
Decomposition temperature/°C	200-360	250-360	270-450	310-450	210-450

Chalone	III				IV	
Form	**III_a**	**III_b**	**III_c**	**III_d**	**IV_a**	**IV_b**
Melting point/°C	120	160	165	156	215.5	215.8
Ethalpy/J·g^{-1}	57.20	71.67	45.45	67.26	76.94	68.8
Decomposition temperature/°C	230-440	280-450	230-450	230-370	290-500	250-500

Table. 3S The maximum absorption and emission peak of all solids

Forms	**I_a**	**I_b**	**II_a**	**II_b**	**II_c**	**III_a**	**III_b**	**III_c**	**III_d**	**IV_a**	**IV_b**
λ^{ab}_{max}/nm	417	492	461	453	442	453	461	486	451	479	518
λ^{em}_{max}/nm	548	/	618	578	611	/	662	551	547	611	/

Table. 4S Contributions of individual intermolecular interactions to the Hirshfeld surface of all crystals

Polymorph	C-H	H-H	O-H	C-C
I_a	33.8%	36.9%	7.6%	6.0%
I_b	35.7%	35.6%	9.3%	3.6%
II_a	42.5%	28.1%	7.3%	6.2%
II_b	26.4%	39.2%	7.8%	12.8%
III_a	41.4%	47.3%	7.4%	3.2%
III_b	39.6%	44.7%	8.1%	6.6%
III_c	26.8%	49.1%	8.4%	15.7%
IV_a	16.4%	35.8%	24.7%	17.3%