Supporting information for:

Single-Benzene Solid Emitters with Lasing Properties based on Aggregation-induced Emissions

Baolei Tang, Huapeng Liu, Feng Li, Yue Wang and Hongyu Zhang*

State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, 2699 Qianjin Avenue, Changchun, P. R. China. Email: <u>hongyuzhang@jlu.edu.cn</u> **Instrumentation:** UV–vis absorption spectra were recorded by a Shimadzu UV-2550 spectrophotometer with or without an integrating sphere. The emission spectra were recorded by a Shimadzu RF-5301 PC spectrometer or a Maya2000 Pro CCD spectrometer. The absolute fluorescence quantum yields of crystals were measured on Edinburgh FLS920 by using an integrating sphere. The fluorescence lifetimes were measured on Edinburgh FLS920 using a time-correlated single-photon (TCSPC) module. The edge emission and PL spectra of the crystals was detected using a Maya2000 Pro CCD spectrometer. The polarization of light emitted from the edge of the crystal was measured by rotating a polarizer. The gain coefficients are measured by adjusting a slit. All the measurements were carried out at room temperature under ambient conditions. Differential scanning calorimetric (DSC) measurements were performed on a NETZSCH DSC204 instrument at a heating rate of 10 °C min⁻¹ under nitrogen. Thermogravimetric analyses (TGA) were performed on a TAQ500 thermogravimeter at a heating rate of 10 °C min⁻¹ under nitrogen.

Single crystal structure: Single crystal X-ray diffraction data were collected on a Rigaku RAXIS-PRID diffractometer using the ω -scan mode with graphitemonochromator Mo K α radiation. The structures were solved with direct methods using the SHELXTL programs and refined with full-matrix leastsquares on *F*₂. Nonhydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated and refined isotropically. The crystallographic information has been deposited with Cambridge Crystallographic Data Centre, and signed to CCDC code 1470379 for **1**, 1470380 for **2**, 1470381 for **3**, and 1470382 for **4**.



Fig. S1 DSC (a) and TGA (b) curves of compounds 1–4.



Fig. S2 Absorption and emission spectra of compounds 1–4 doped in PMMA films (5 wt%).



Fig. S3 Emission spectra of crystalline samples 1–4.



Fig. S4 Time-resolved photoluminescent dynamic of crystals 1–4.



Fig. S5 Molecular packing structure and hydrogen-bonding interactions of crystal 1.



Fig. S6 Molecular packing structure and hydrogen-bonding interactions of crystal 4.



Fig. S7 The hydrogen-bonding interactions of the molecules A and B in crystal 2.



Fig. S8 PL spectra as the function of the pump laser energy (a) and the pump laser energy dependent peak intensity and FWHM (b) of crystal 1.



Fig. S9 PL spectra as the function of the pump laser energy (a) and the pump laser energy dependent peak intensity and FWHM (b) of crystal **3**.



Fig. S10 PL spectra as the function of the pump laser energy (a) and the pump laser energy dependent peak intensity and FWHM (b) of crystal 4.



Fig. S11 (a) Peak intensity of PL spectra as a function of the pump stripe length at different pump energies and (b) the net gain coefficient as a function of wavelength at different pump energies of crystal **1**.



Fig. S12 Dependence of the intensity of polarized light from crystal 1 on the relative polarization angle φ .