Supporting Information

Aggregation-Induced Emission on Benzothiadiazole Dyads with Large Third-Order Optical Nonlinearity

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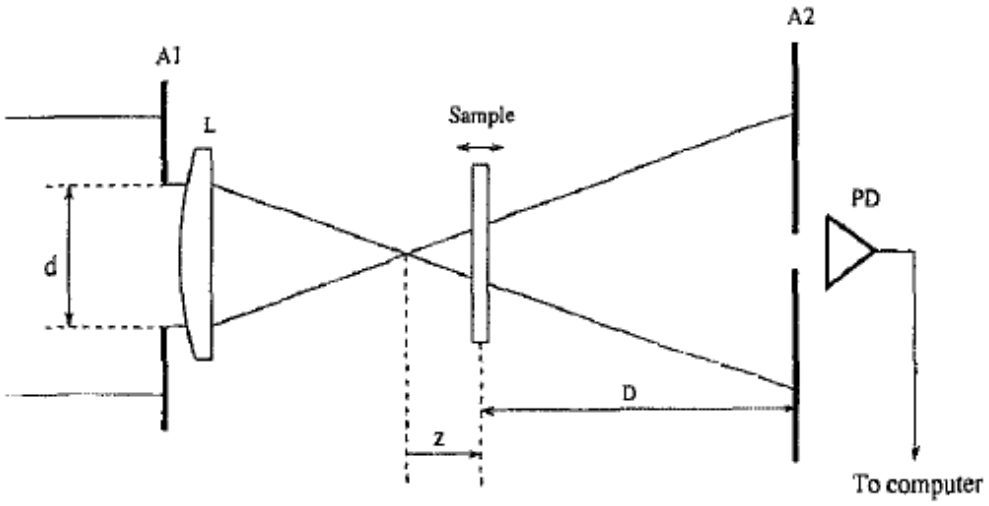

Figure S1. The schematic of the Z-scan setup.A1, A2: apertures; L: lens with focal length f; PD: photodetector.

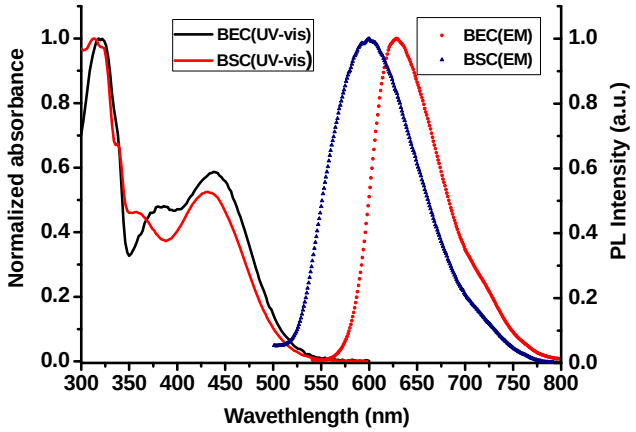

Figure S2. Absorbance (in CH_2Cl_2) and fluorescence (in the film) spectra of **BEC** and **BSC**.

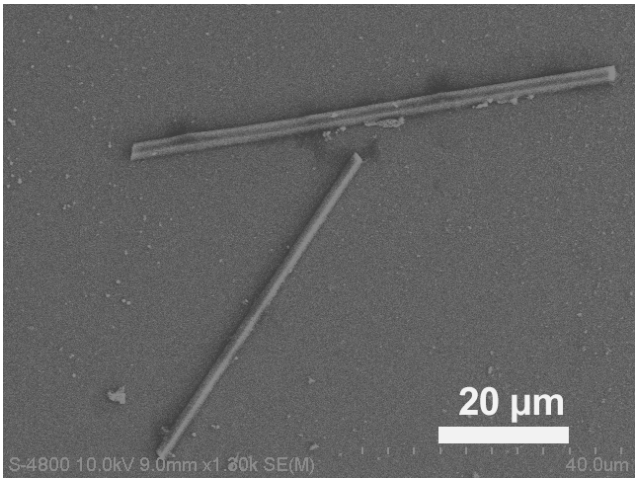

Figure S3 .Microrods structures of **BEC**.

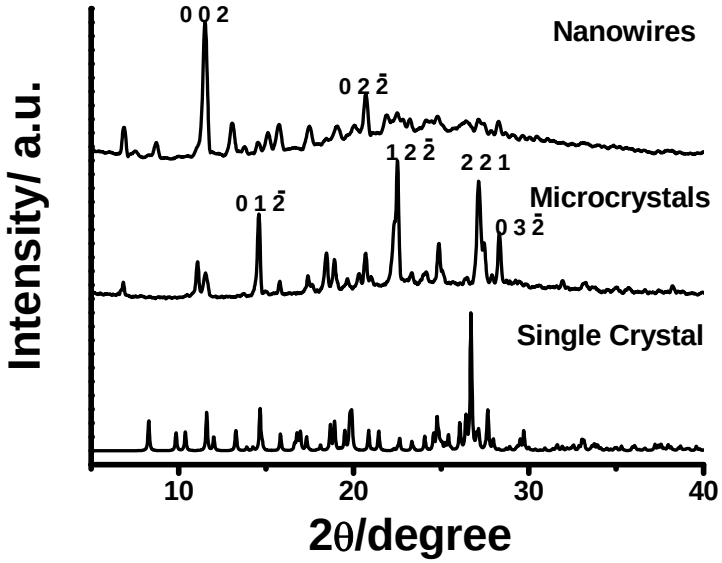

Figure S4. Powder XRD patterns of **BEC**, the single-crystal (bottom), as-prepared microcrystals (middle) and nanowires (top).

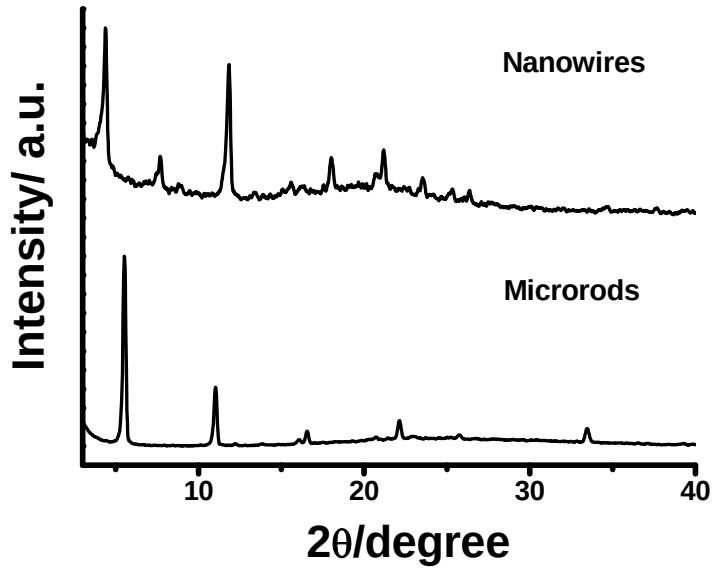

Figure S5. Powder XRD patterns of **BSC**, the microrods (bottom) and nanowires (top).

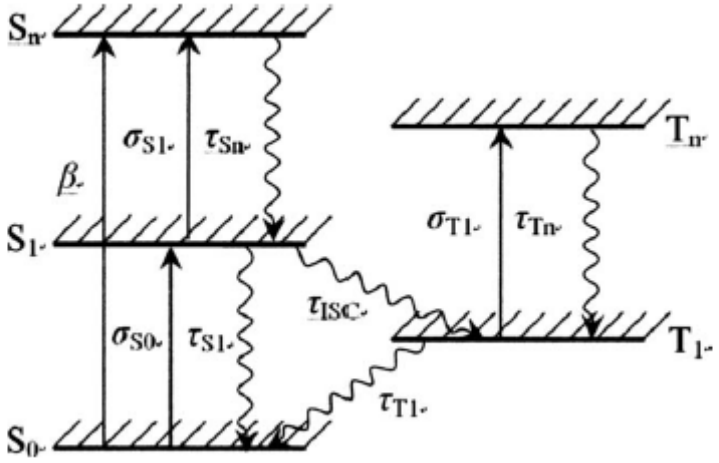

Figure S6. Energy-level diagram of **BEC** molecule.

$$NT = \frac{E_{nl}}{E_l} = \frac{2\pi \int_{-\infty}^{+\infty} dt \int_0^{\infty} r I_{pL} dr}{E_0 T_0} \quad \textbf{(4)}$$

$$\frac{dI_p}{dz} = -(\sigma_{S0} N_{S0} + \sigma_{S1} N_{S1} + \sigma_{T1} N_{T1} + 2\beta I_e) I_p \quad \textbf{(5)}$$

$$\frac{d\varphi_p}{dz} = k(\Delta\eta_{S1} N_{S1} + \Delta\eta_{T1} N_{T1} + 2n_2 I_e) \quad \textbf{(6)}$$

$$\frac{dI_e}{dz} = -(\sigma_{So} N_{So} + \sigma_{S1} N_{S1} + \sigma_{T1} N_{T1} + \beta I_e) I_e \quad \textbf{(7)}$$

$$\frac{dN_{S0}}{dt} = -\frac{\sigma_{So} I_e N_{So}}{\hbar\omega} - \frac{\beta I_e^2}{2\hbar\omega} + \frac{N_{S1}}{\tau_{S1}} + \frac{N_{T1}}{\tau_{T1}} \quad \textbf{(8)}$$

$$\frac{dN_{S1}}{dt} = -\frac{\sigma_{S1} I_e N_{S1}}{\hbar\omega} + \frac{\sigma_{S0} I_e N_{S0}}{\hbar\omega} - \frac{N_{S1}}{\tau_{S1}} - \frac{N_{S1}}{\tau_{ISC}} + \frac{N_{Sn}}{\tau_{Sn}} \quad \textbf{(9)}$$

$$\frac{dN_{Sn}}{dt} = \frac{\sigma_{S1} I_e N_{S1}}{\hbar\omega} + \frac{\beta I_e^2}{2\hbar\omega} - \frac{N_{Sn}}{\tau_{Sn}} \quad \textbf{(10)}$$

$$\frac{dN_{T1}}{dt} = -\frac{\sigma_{T1} I_e N_{T1}}{\hbar\omega} - \frac{N_{T1}}{\tau_{T1}} + \frac{N_{S1}}{\tau_{ISC}} + \frac{N_{Tn}}{\tau_{Tn}} \quad \textbf{(11)}$$

$$\frac{dN_{Tn}}{dt} = -\frac{\sigma_{T1} I_e N_{T1}}{\hbar\omega} - \frac{N_{Tn}}{\tau_{Tn}} \quad \textbf{(12)}$$

Figure S7. Equations used to calculate the nonlinear data.

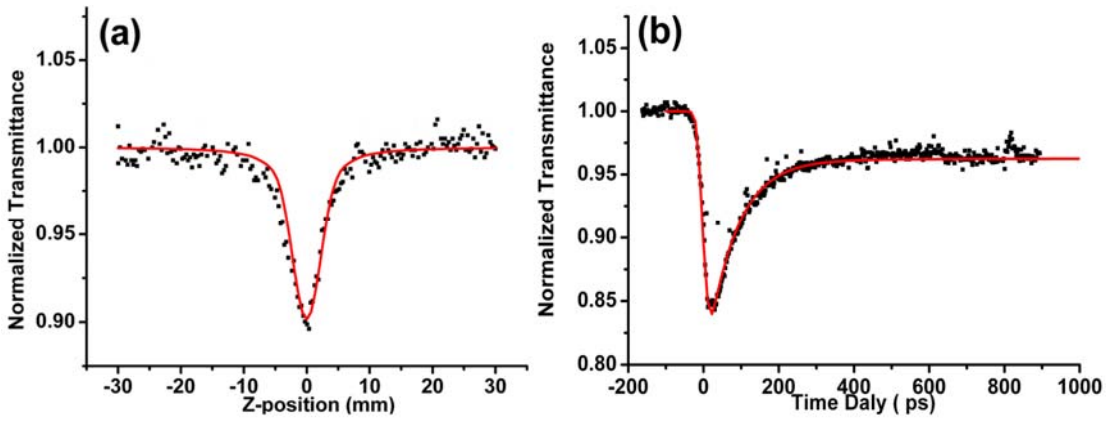

Figure S8. Normalized open-aperture Top-hat Z-scan curves (a) and Pump-probe curves of nonlinear absorbance (b) of **BSC**.