Supporting information

Enhanced Photoinduced Electron Transfer and Stability of Diradicals in Neutral Extended Pyridine N-Oxides

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1. **Experimental materials.**

All the chemicals were purchased commercially and used without further treatment.

2. **Experimental methods.**

Infrared (IR) data were obtained by a PerkinElmer Spectrum One FT-IR spectrophotometer over the scope 4000–400 cm\(^{-1}\) with the pure KBr pellets as the baseline. \(^1\)H-NMR spectra were measured at room temperature by an Advance III NMR spectrometer operating at 400 MHz. Solid-state \(^{13}\)C-NMR spectra were measured at room temperature by an Advance III HD NMR spectrometer operating at 400 MHz. Electronic absorption spectra were measured in the reflectance mode at room temperature on a Perkin-Elmer Lambda 900 UV/vis/NIR spectrophotometer with an integrating sphere attachment and BaSO\(_4\) as a reference. Photoluminescent spectra were recorded on a single-grating Edinburgh EI920 fluorescence spectrometer equipped with a 450 W Xe lamp. Electron spin resonance (ESR) spectra were recorded on a Bruker ER-420 spectrometer with a 100 kHz magnetic field in the X band. Thermogravimetric (TG) analyses were performed on a NETZSCH STA 449C simultaneous thermal analyzer with Al\(_2\)O\(_3\) crucibles under N\(_2\) (20 mL·min\(^{-1}\)) at a heating rate of 10 K·min\(^{-1}\). Powder X-ray diffraction pattern (PXRD) patterns were collected at room temperature on a Rigaku MiniFlex II diffractometer using Cu K\(\alpha\) radiation (\(\lambda = 1.5406\) Å). Simulated PXRD patterns were derived from the Mercury Version 3.5.1 software using the X-ray single crystal diffraction data. Light source: A PLSSXE300C 300 W xenon lamp system equipped with an IR filter was used to illuminate samples for achieving various spectra, and the distances between these samples and the Xe lamp were around 25 cm.
The density functional theory (DFT) method was employed to perform all the calculations. All geometry optimizations and calculations for reduced density gradient (RDG) isosurfaces were conducted at the b3lyp/6-31g(d,p) level. Calculation for electrostatic potentials (ESP) and interaction energy were performed at the M06-2x/6–311G(d,p) level. The Gaussian 09 package[1] was used for all above calculations.

Reference:

3. Additional graphics

**Figure S1.** $^1$H-NMR spectrum of the as-synthesized sample of BPDO in $d_6$-DMSO.

**Figure S2.** IR spectra of the BPDO powder before and after irradiation in the KBr matrix.
Figure S3. ESR spectrum of DPPH (10 mg) in the solid state at room temperature.

Figure S4. $^1$H-NMR spectra of the as-synthesized sample, irradiated sample in argon and irradiated sample in air of BPDO in $d_6$-DMSO.
Figure S5. IR spectra of the BPTDO powder before and after irradiation in the KBr matrix.

Figure S6 TG curve for the BPDO powder.
Figure S7. PXRD pattern for the BPDO powder. For comparison, the simulated pattern derived from the single-crystal diffraction data of BPDO·2H₂O is also shown.

Figure S8. Gradient isosurfaces (s = 0.5 a.u.) for one tetramer truncated from the crystal structure of BPDO·2H₂O (calculated at b3lyp/6-31g(d,p) level). The surfaces are colored on a blue-green-red (BGR) scale according to values of sign(λ₂)ρ, ranging from −0.04 to 0.02 a.u.. Blue indicates strong attractive interactions, and red indicates strong nonbonded overlap.
Figure S9. Fluorescence emission spectra of the BPDO powder before and after irradiation.

Figure S10. Fluorescence emission spectra of the BPTDO powder before and after irradiation.

Table S1. Interaction energies $\Delta E$ of BPDO aggregates calculated at the M06-2X/6-311G(d,p)
level with BSSE correction. Vertical and horizontal directions indicate packing directions through $\pi-\pi$ interactions and C–H–O bonds, respectively. Cartesian coordinates and structures of BPDO aggregates are listed below this table.

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![Image of Cartesian coordinates and structure of one trimer]

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**Table S2.** Calculated spin population at the b3lyp/6-31g** level for open-shell singlet state and triplet diradical in vacuum.

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