Electronic Supplementary Material (ESI) for RSC Advances.


# Efficient solid-state emission and reversible mechanofluorochromism of tetraphenylethene-pyrene-based β-diketonate boron complex

Ting Sun [a], Feng Zhao [a, b, *], Gaolei Xi [c], Mengyu Sun [a], Jian Gong [a], Chang Dong [a], Jingyi Qiu [a]

[a] *College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang 455000, P. R. China*

[b] *Henan Province Key Laboratory of New Opto-Electronic Functional Materials, Anyang 455000, P. R. China*

[C] *Technology Ceter, China Tobacco Henan Industrial Co., Ltd., Zhengzhou 45000, P.R. China*

** Corresponding author. E-mail addresses: zhaofeng@aynu.edu.cn*

## Table of Contents

**Table S1**. Photophysical data of **$BF_2$-TP** in different solvents.

| solvent | $\lambda_{abs}$/nm (ε/mol$^{-1}$ cm$^{-1}$) | $\lambda_{em}$/nm | $\Delta\nu_{st}$[a]/cm$^{-1}$ | $\Phi_f$[b] |
|---|---|---|---|---|
| hexane | 324 (25800), 340 (28000), 411 (22000), 438 (19400) | 507 | 4548 | 0.369 |
| cyclohexane | 325 (35600), 341 (39000), 414 (29500), 442 (25600) | 511 | 4585 | 0.354 |
| toluene | 327 (35600), 342 (36100), 420 (25200) | 543 | 5393 | 0.208 |
| THF | 326 (32100), 341 (35800), 419(26000) | 576 | 6448 | 0.196 |
| DCM | 327 (32300), 342 (34700), 424 (24200), 461 (24700) | 609 | 7276 | 0.190 |
| DMF | 327 (32500), 342 (37300), 423 (25700), 465 (22600) | 631 | 7793 | 0.095 |
| DMSO | 331 (32900), 344 (32300), 429 (25300), 456 (25800) | 645 | 7806 | 0.083 |

[a]$\Delta\nu_{st} = \nu_{abs}-\nu_{em}$. [b]The fluorescence quantum yield ($\Phi_f$) was measured using fluorescein ($\Phi$ = 0.79 in 0.1 M sodium hydroxide water solution) as standard.

**Table S2**. Solid-state fluorescence lifetime data of **$BF_2$-TP** samples in as-prepared and grinding state

| | as-prepared | grinding |
|---|---|---|
| $\tau_1$ [a] (ns) | 3.03 | 3.18 |
| $\tau_2$ [a] (ns) | 9.59 | 9.57 |
| $A_1$ [b] (%) | 91.12 | 31.28 |
| $A_2$ [b] (%) | 8.88 | 68.72 |
| $\tau_f$ [c] (ns) | 3.61 | 7.57 |
| $\Phi_f$ [d](%) | 45.90 | 34.88 |
| $k_f$ [e]($s^{-1}$) | $1.27\times10^8$ | $4.61\times10^7$ |
| $k_{nr}$ [f]($s^{-1}$) | $1.50\times10^8$ | $8.60\times10^7$ |

[a] Fluorescence lifetime. [b] Fractional contribution. [c] Weighted mean lifetime.

[d] The fluorescence quantum yield, $\lambda_{ex}$ = 370 nm. [e] Radiative ($k_f = \Phi_f/\tau_f$).

[f] Nonradiative rate constants ($k_{nr} = (1-\Phi_f)/\tau_f$).

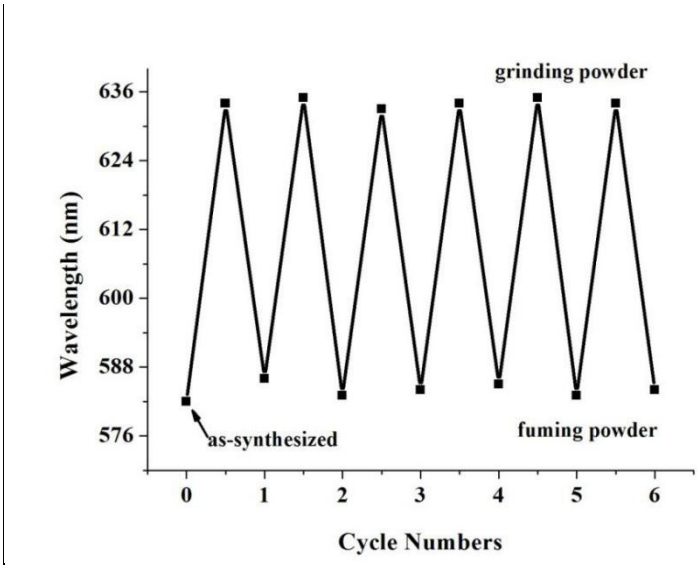


**Fig. S1** Maximum fluorescent emission of **$BF_2$-TP** upon repeating treatment by grinding and fuming with DCM vapor.

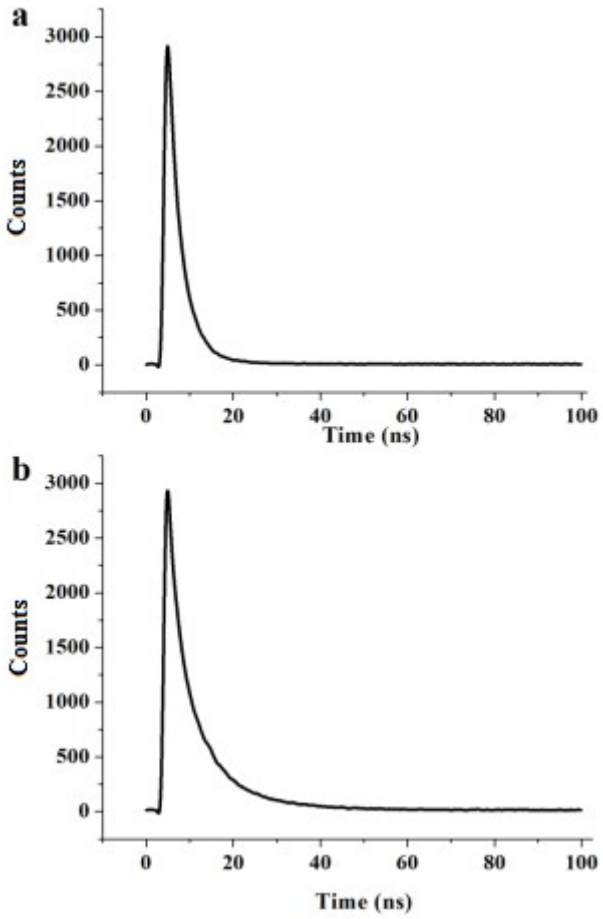


Fig. S2 Fluorescence decay profiles of as-prepared (**a**) and grinding (b) **$BF_2$-TP**, $\lambda_{ex}$ = 370 nm.

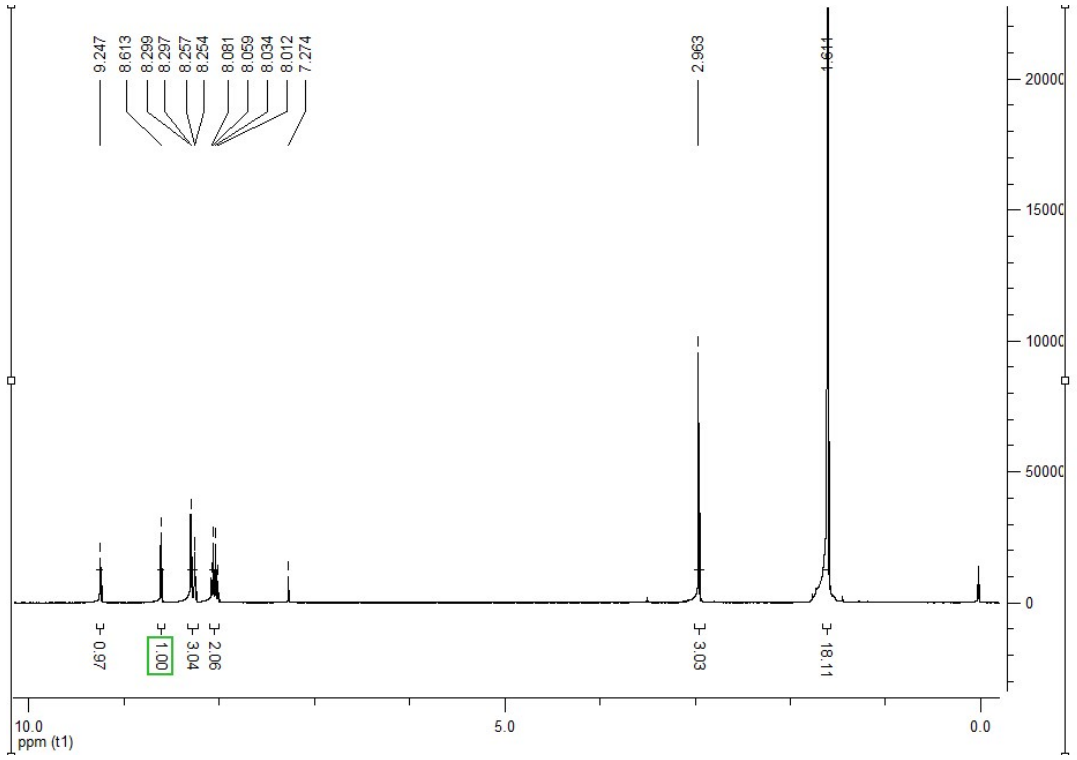


**Fig. S3** $^{1}$H NMR (400 MHz) spectrum of compound **6**.

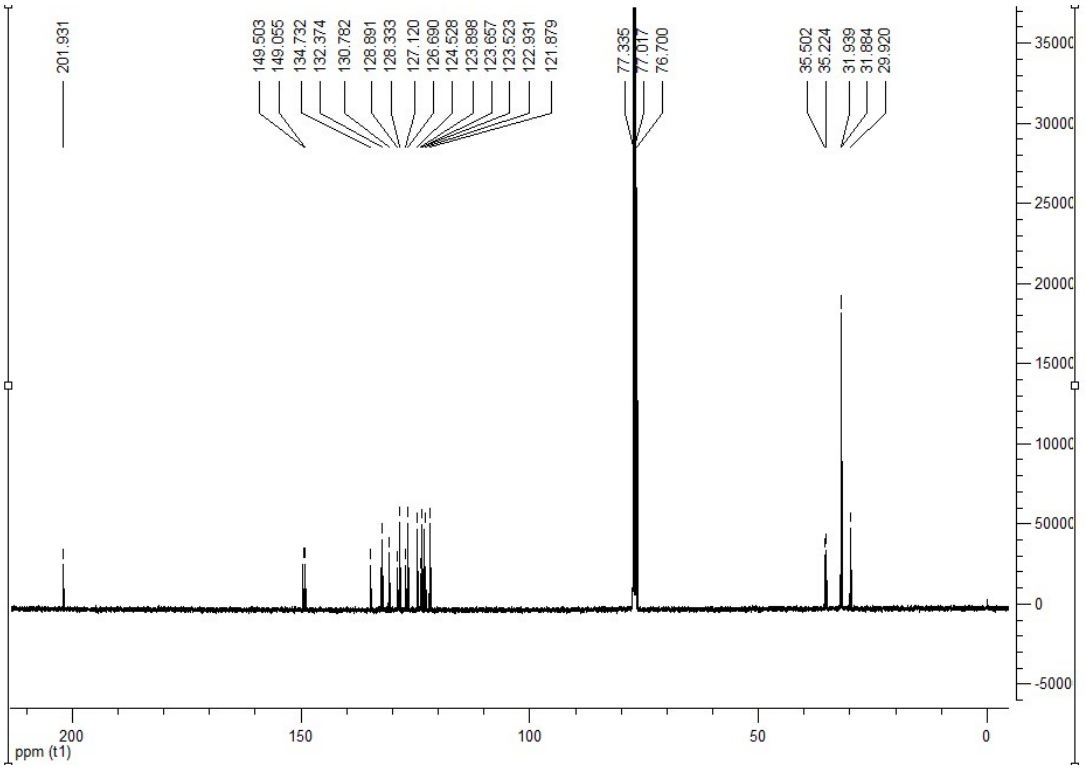

**Fig. S4** $^{13}$C NMR (100 MHz) spectrum of compound **6**.

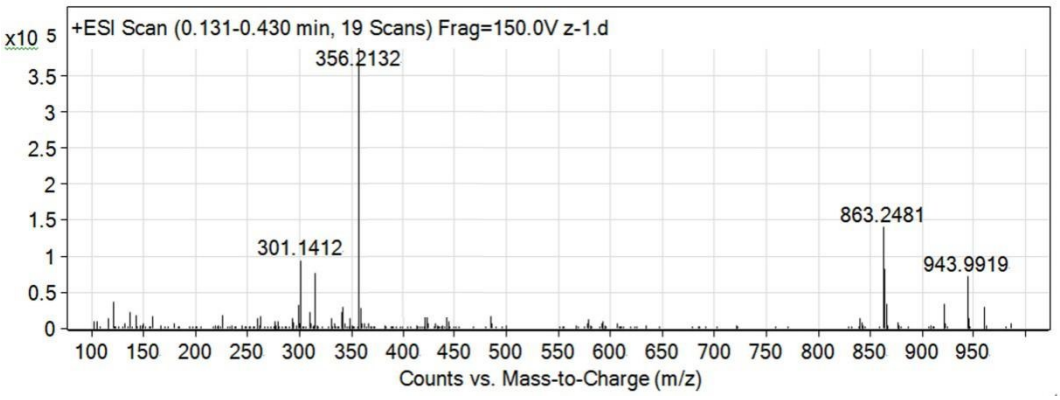


**Fig. S5** TOF LC/MS spectrum of compound **6**.

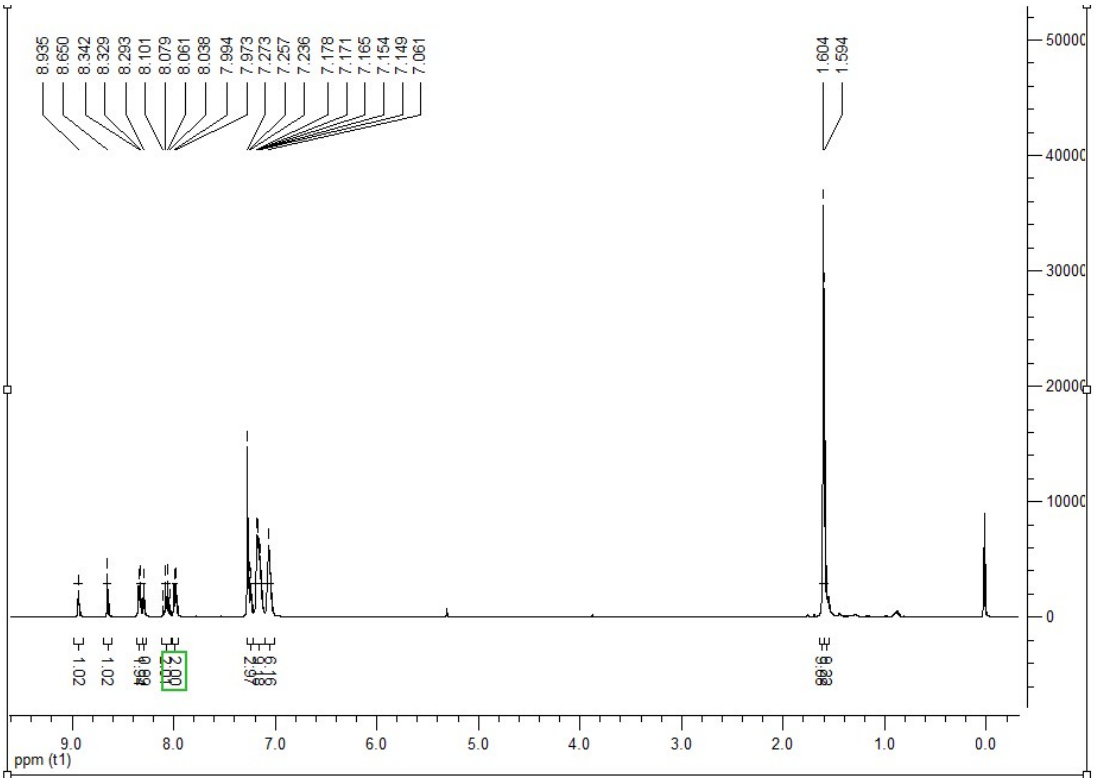


**Fig. S6** $^{1}$H NMR (400 MHz) spectrum of compound **$BF_2$-TP**.

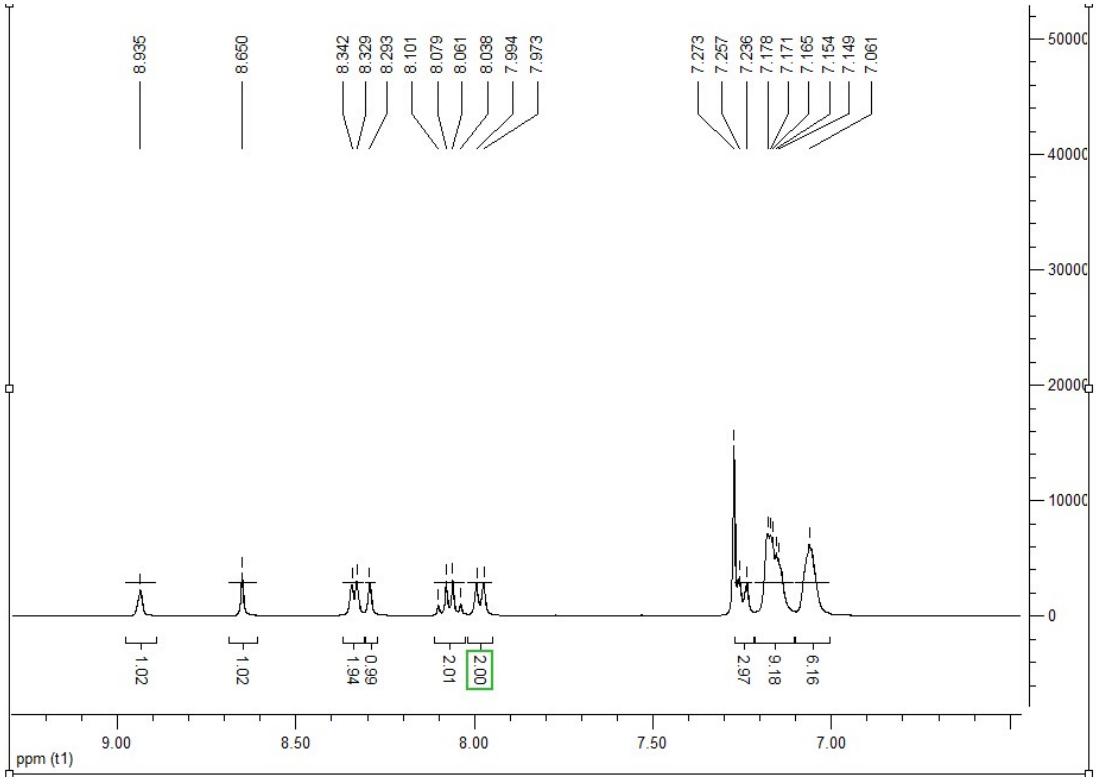


**Fig. S7** $^{1}$H NMR (400 MHz) spectrum (larger version) of compound **$BF_2$-TP**.

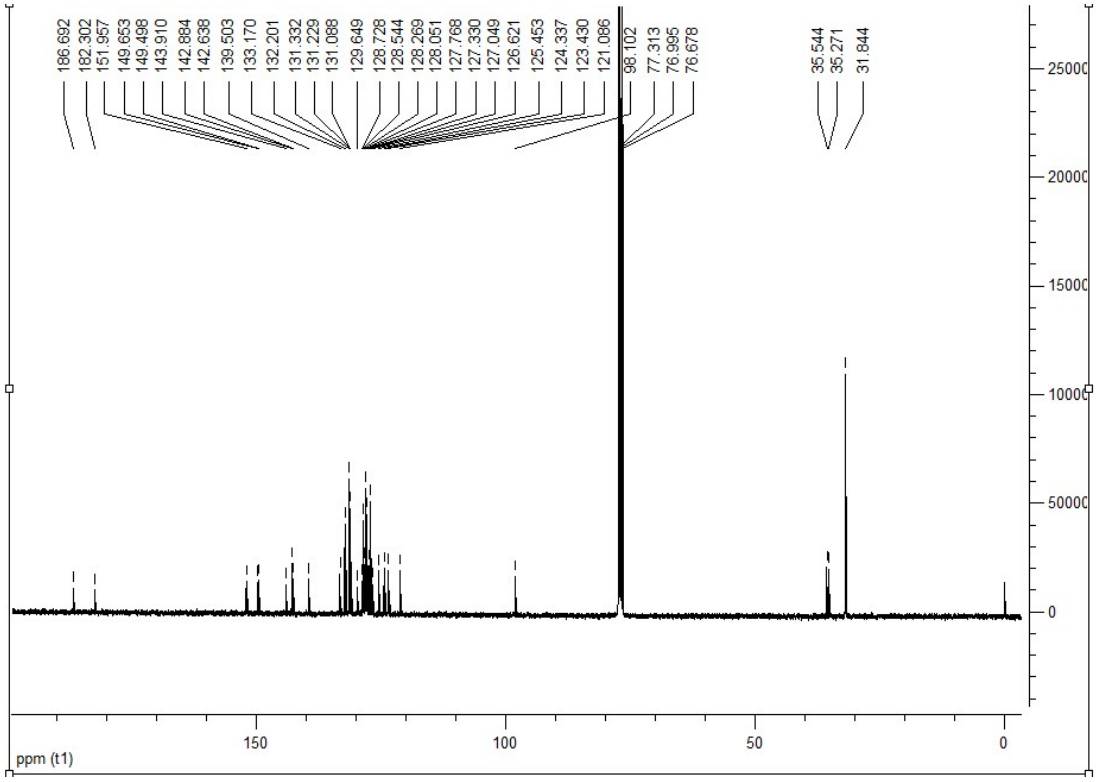


**Fig. S8** $^{13}$C NMR (100 MHz) spectrum of compound **$BF_2$-TP**.

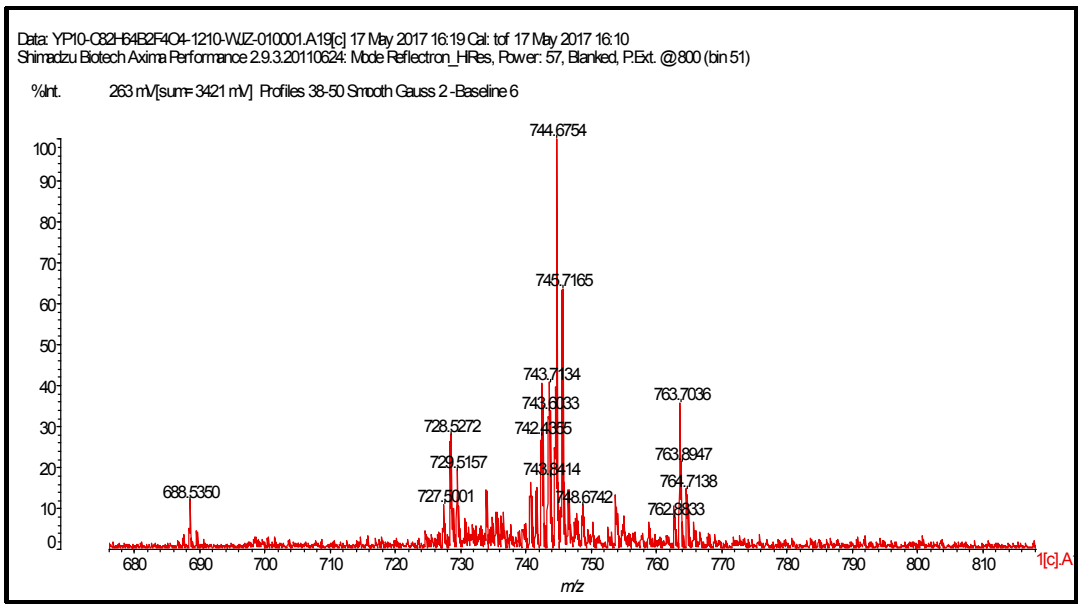


**Fig. S9** MALDI/TOF MS spectrum of compound **$BF_2$-TP**.