Supporting Information

Circularly Polarized Luminescent Systems Fabricated by Tröger's Base Derivatives through Two Different Strategies

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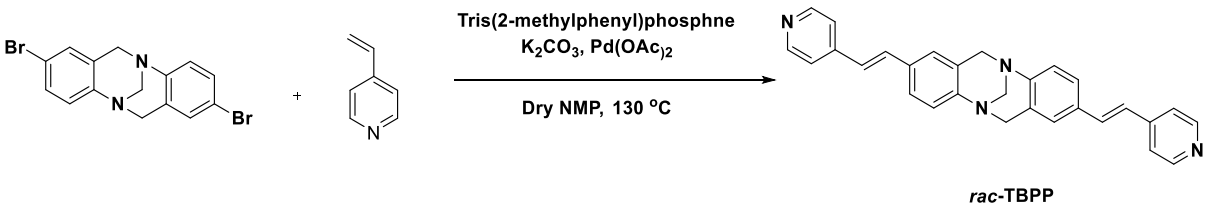
Table of Contents

1. General information

All reactions were performed in air atmosphere unless otherwise stated. All reagents and solvents, unless otherwise indicated, were obtained from commercial sources. Melting points (M.p.) were determined using a Focus X-4 apparatus (made in China) and were not corrected. All yields were given as isolated yields. NMR spectra were recorded on a Bruker DPX 400 MHz spectrometer tetramethylsilane (TMS) solvent signals as internal references at 298 K. LCMS equipped with an electrospray ionization (ESI) probe operate in positive-ion mode with direct infusion. Fourier transform infrared (FT-IR) spectra were recorded using a Thermo Nicolet Nexus FT-IR devise with the Smart Golden Gate ATR attachment in the range of 4000-400 cm^{-1} with 2 cm^{-1} resolution. UV-vis and CD spectra were obtained using Hitachi U-3600 spectrophotometer and JASCO J-810 spectrophotometer, respectively. Fluorescence spectra of both the solution and cogels were measured on a F-7000 FL spectrophotometer (HITACHI, Japan) using a xenon lamp as the excitation source. CPL spectra were measured on JASCO CPL-300.

2. Synthesis of *rac*-TBPP and the gelator DGG



Scheme S1. The synthesis procedures of ***rac*-TBPP**.

Synthesis of *rac*-TBPP and characterization data

2,8-dibromo-6H,12H-5,11-methanodibenzo[b,f][1,5]diazocine was initially synthesized according to the reported procedures [S1]. *rac*-**TBPP** was synthesized according to the reported literature [S2]. A single-necked flask equipped with a magnetic stirrer was charged with 2,8-dibromo-6H,12H-5,11-methanodibenzo[b,f] [1,5]diazocine (0.667 mmol, 0.252 g), K_2CO_3 (3.76 mmol, 0.52 g), tris(2-methylphenyl) phosphine (1.0 mmol, 0.30 mg) and palladium acetate (1.0 mmol, 2.25 mg) in dry N-methyl pyrrolidone solution (10 mL) under an N_2 atmosphere. Then 4-vinyl pyridine (2.13 mmol, 0.22ml) was added slowly by using a syringe, and the solution was refluxed at 130 °C for 12h. After the reaction was finished, the reaction mixture was cooled to ambient temperature and extracted by CH_2Cl_2 (3 × 100 mL). The organic phase was washed with saturated sodium chloride solution and dried with anhydrous Na_2SO_4. After being filtered, the organic solvent was removed using rotary evaporator, the product was purified by column chromatography on silica gel (eluent: 1/40, *v/v*, methanol :

dichloromethane gradually changing to 1/25) to afford *rac*-**TBPP** as a yellow solid (0.147 g, 0.345 mmol, 51.8 %). M. p.: 286-288 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.54 (d, J = 6.0 Hz, 4H), 7.38 (dd, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 2H), 7.34-7.32 (m, 4H), 7.21-7.10 (m, 6H), 6.87 (d, J = 16.4 Hz, 2H), 4.75 (d, J = 16.4 Hz, 2H), 4.35 (s, 2H), 4.24 (d, J = 16.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): 149.1, 148.6, 146.2, 133.8, 131.8, 128.2, 126.3, 126.0, 125.5, 124.5, 121.0, 66.9, 58.7 ppm. (ESI-MS) m/z: calcd. for $[C_{29}H_{24}N_4 + H]^+$ = 429.20; found: 429.05.

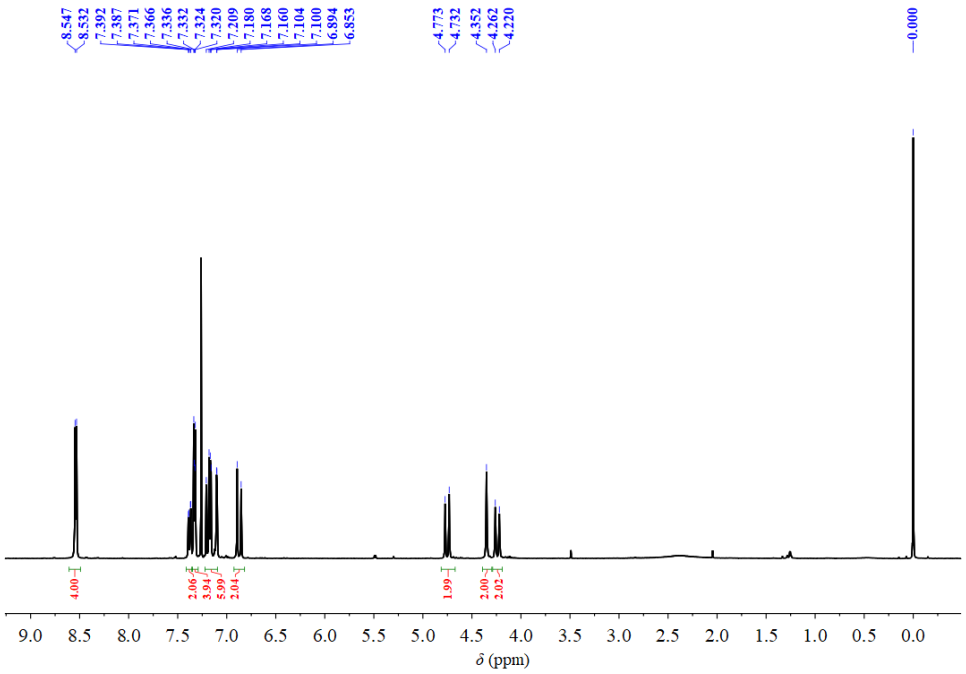


Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of *rac*-**TBPP**.

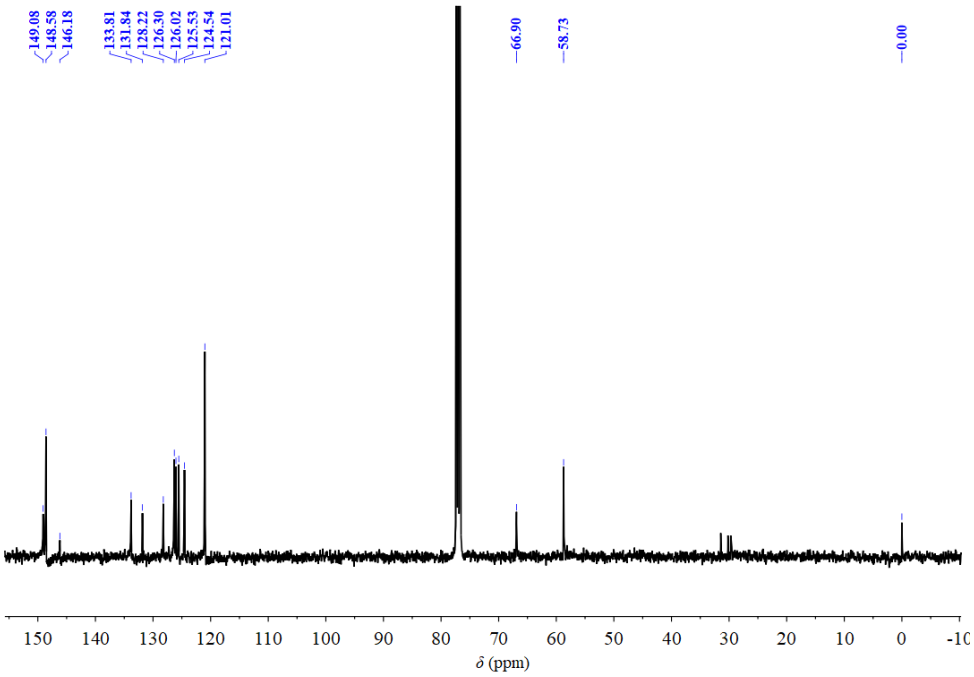


Figure S2. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of *rac*-**TBPP**.

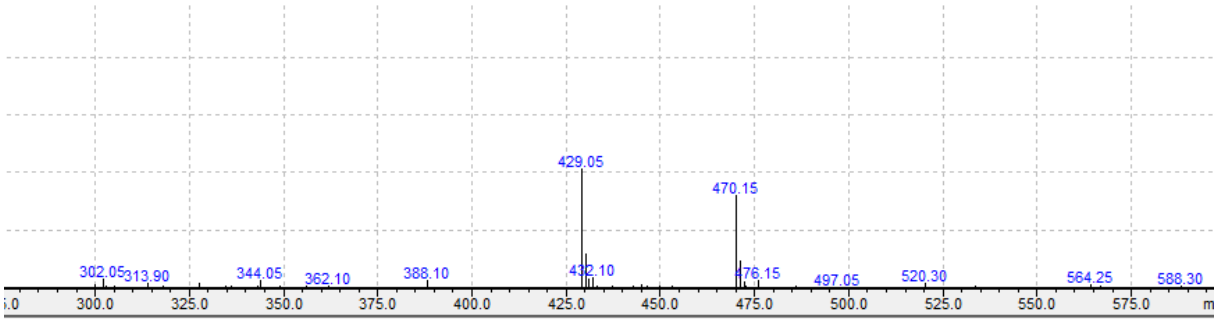
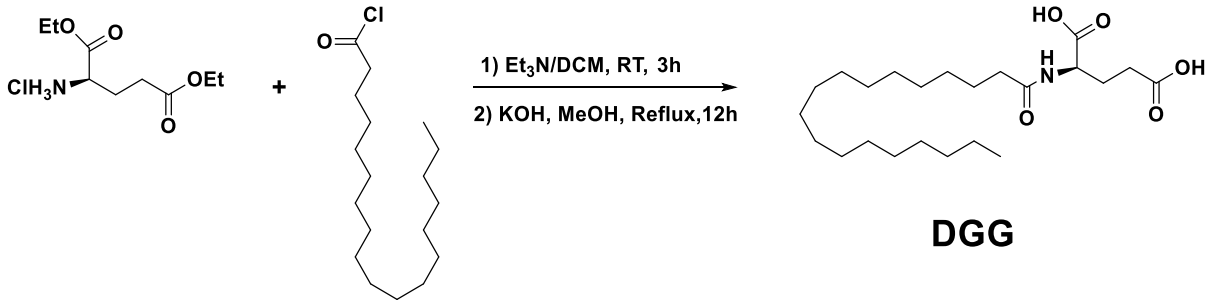


Figure S3. ESI-MS of ***rac*-TBPP** with the parent ion $[M+H]^+$ at 429.05



Scheme S2. The synthesis procedures of **DGG**.

Synthesis of the gelator DGG/LGG and characterization data

DGG was prepared according to the previously reported methods [S3].

The compound *L*-glutamic acid diethyl ester hydrochloride (1,02 g, 4.26 mmol) was dissolved in dry CH_2Cl_2 (80 mL) containing Et_3N (1.24 g, 1.61 mL, 12.25 mmol) at 0 °C, and a solution of stearoyl chloride (1.38 ml, 5.01 mmol) in dry CH_2Cl_2 (20 mL) was added to the mixture slowly over 1h. After warming to ambient temperature, the mixed solution was stirred for additional 3h. Then the reaction was quenched by addition of deionized water (100 mL), and extracted by CH_2Cl_2 (2 × 100 mL), the organic phase was dried with anhydrous Na_2SO_4. The crude product was obtained after filtration and rotary evaporation. The product was used for next step without purification, which was dissolved in a 1:1 mixture solution of MeOH/water (*v*/*v*, 80 mL) and KOH (0.32 g, 5.70mmol) was added. The mixture was heated under reflux for 12h. After cooling to ambient temperature, MeOH was removed using rotary evaporator, and the aqueous phase was acidified with 2M HCl to pH = 2.0. The formed precipitate was filtered off, washed with deionized water thoroughly, dried and recrystallized using acetone as solvent to obtain the white solid (1.38 g, 3.34 mmol, 78.6 %). ^{1}H NMR (400 MHz, DMSO-d_6) δ = 12.32 (s, 2H), 8.04 (d, J = 8.0 Hz, 1H), 4.21-4.16 (m, 1H), 2.28-2.24 (m, 2H), 2.12-2.08 (m, 2H), 1.99-1.90 (m, 1H), 1.79-1.70 (m, 1H), 1.49-1.46 (m, 1H), 1.23 (s, 28H), 0.85 (t, J = 6.4 Hz, 3H) ppm. **LGG** was obtained by the same synthetic procedure as above-mentioned for **DGG**.

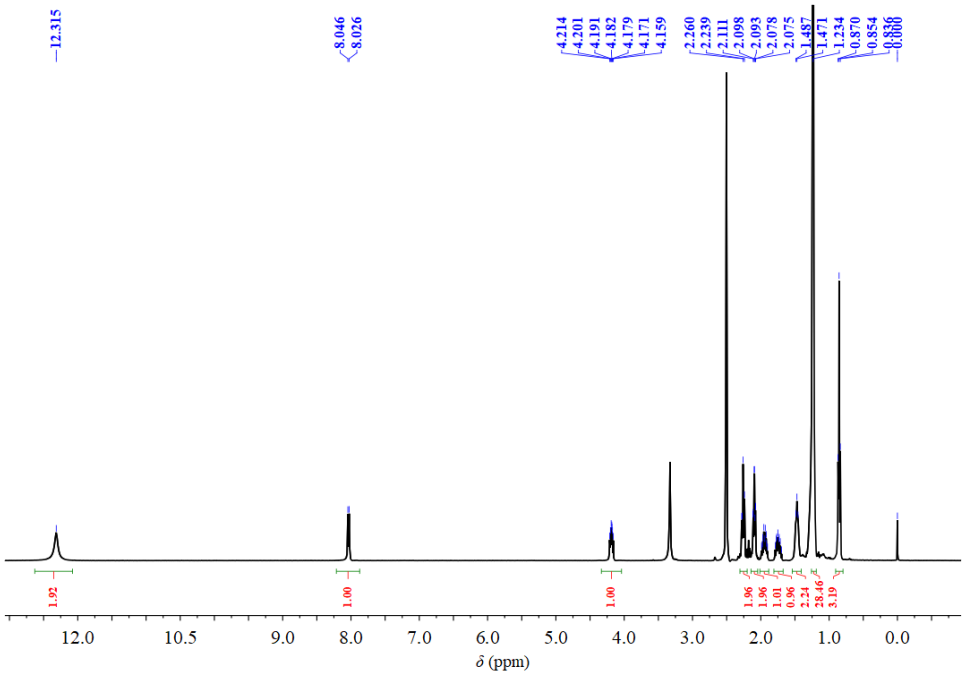
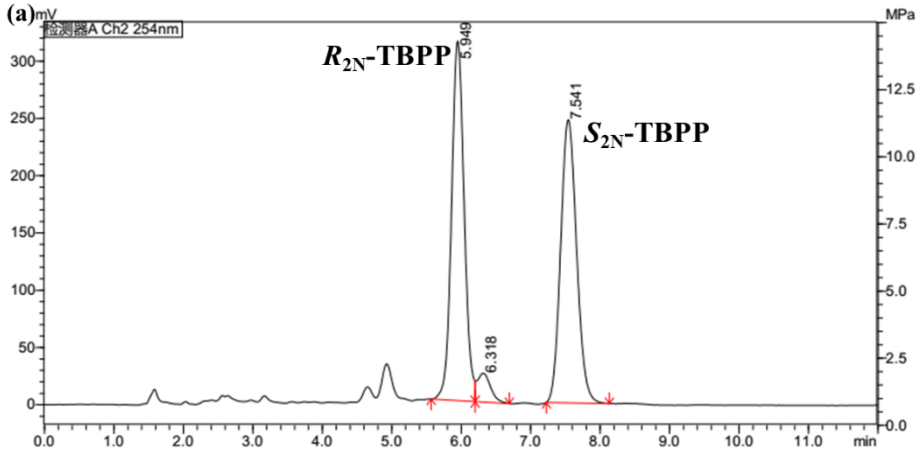


Figure S4. ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of **DGG**.

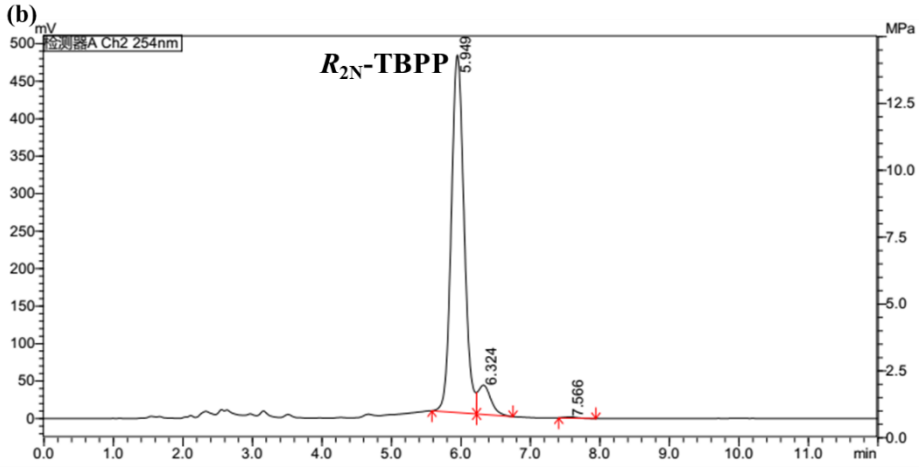
3. Chiral resolution of *rac*-TBPP by chiral HPLC.

Optical isomer resolution conditions:

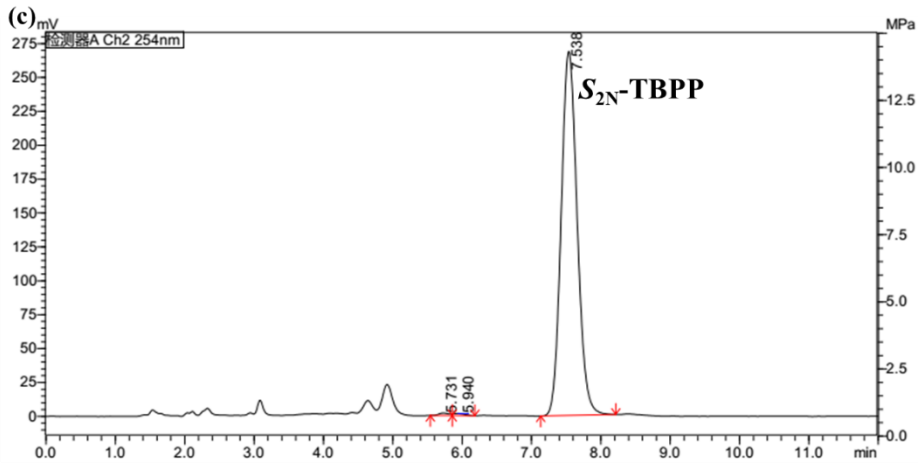
Column	:	CHIRALPAK IB N-5(IBN5CD-VD005)
Column size	:	0.46 cm I.D. × 15 cm L
Injection	:	20.0 ul
Mobile phase	:	MeOH/DCM=80/20(V/V)
Flow rate	:	1.0 ml/min
Wave length	:	UV 25 nm
Temperature	:	35 ºC
HPLC equipment	:	Shimadzu LC-20AD CP-HPLC-06
Sample name	:	Raw Material



Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	5.949	3970818	48.181	5031	--	--
2	6.318	331918	4.027	2794	--	0.907
3	7.541	3938691	47.791	5083	1.117	2.715



Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	5.949	6120274	92.261	4906	--	--
2	6.324	496936	7.491	2571	--	0.895
3	7.566	16471	0.248	7663	1.185	2.941



Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	5.731	19446	0.448	4450	--	--
2	5.940	15549	0.358	2946	--	0.537
3	7.538	4307267	99.194	5003	1.116	3.697

Figure S5. Resolution of the enantiomers [***R*$_{2N}$-TBPP** and ***S*$_{2N}$-TBPP**] of ***rac*-TBPP** by a preparative chiral HPLC (a) ***rac*-TBPP**, (b) ***R*$_{2N}$-TBPP**, (c) ***S*$_{2N}$-TBPP**.

4. Fabrication of the cogels

DGG (20.0 mg, 48.0 mmol) was added to a capped test tube with **TBPP** (3×10^{-3} M for 1:16 and 4.8×10^{-4} M for 1:100) chloroform solution (1.0 mL), the mixture was heated until the solid was dissolved completely. The solution was subsequently cooled down to room temperature. After 10 min, the gel formed and determined by the absence of flow of the solvent when the tube was inverted [S4].

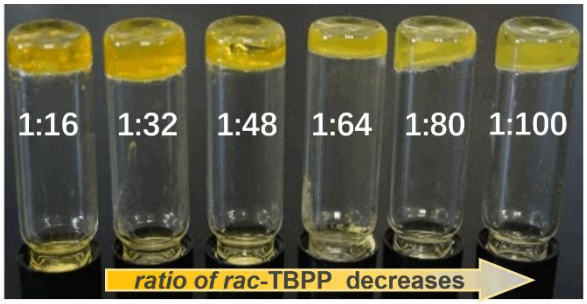


Figure S6. Cogels at different stoichiometric ratios of ***rac*-TBPP/DGG.**

5. FT-IR absorption spectra of *rac*-TBPP/DGG cogels

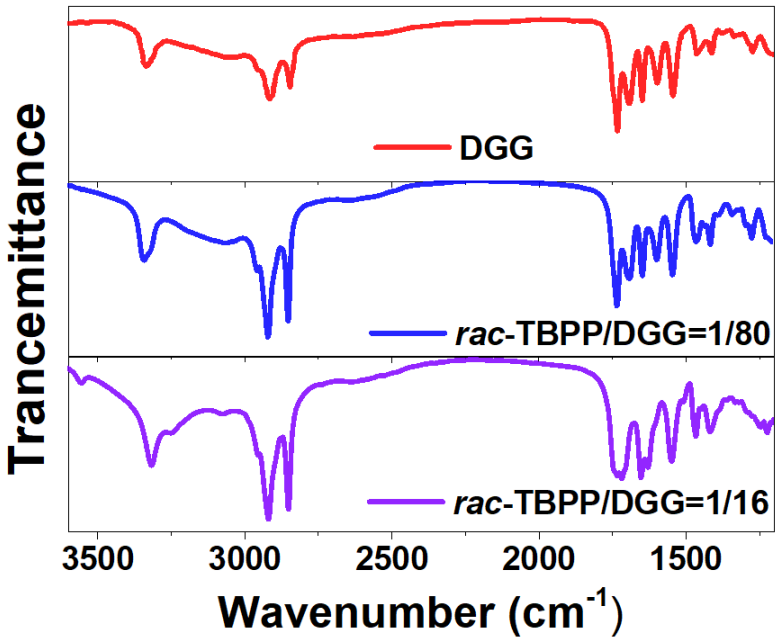


Figure S7. FT-IR absorption spectra of ***rac*-TBPP/DGG** cogels at molar ratios of 1 : 80 and 1:16.

6. Reference

S1. Hu, X.; He, Y.; Wang, Z.; Yan, J. *Polymer* **2018**, *153*, 173-182. doi: 10.1016/j.polymer.2018.08.013

S2. Yuan, C.; Zhang, Y.; Xi, H.; Tao, X. *RSC Adv.* **2017**, *7*, 55577-55581. doi:10.1039/c7ra11228a

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S4. Li, P.; Lue, B.; Han, D.; Duan, P.; Liu, M.; Yin, M. *Chem. Commun.* **2019**, *55*, 2194-2197. doi:10.1039/c8cc08924h