A Boron-Containing Carbazole Dimer: Synthesis, Photophysical Properties and Sensing Properties

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Electronic Supplementary Information (ESI†)

Contents

Compound	Excitation energy (eV)	λ_{abs} (nm)	Oscillator strength (f)	Main configurations	
BCCB	2.9384	421.94	0.9967	HOMO→LUMO	0.68
	3.5222	352.01	0.5279	HOMO→LUMO+2	0.47
				HOMO→LUMO+3	0.29
	3.5992	344.48	0.8105	HOMO→LUMO+3	0.56
				HOMO→LUMO+2	-0.32
	3.7533	330.34	0.5398	HOMO-1→LUMO+1	0.36
				HOMO→LUMO+2	0.32
				HOMO-2→LUMO	0.29

Table S1 The electronic transition data obtained by TD-DFT/ B3LYP/6-31G (d, p) method for the optimized geometry of compound **BCCB** in the ground state.

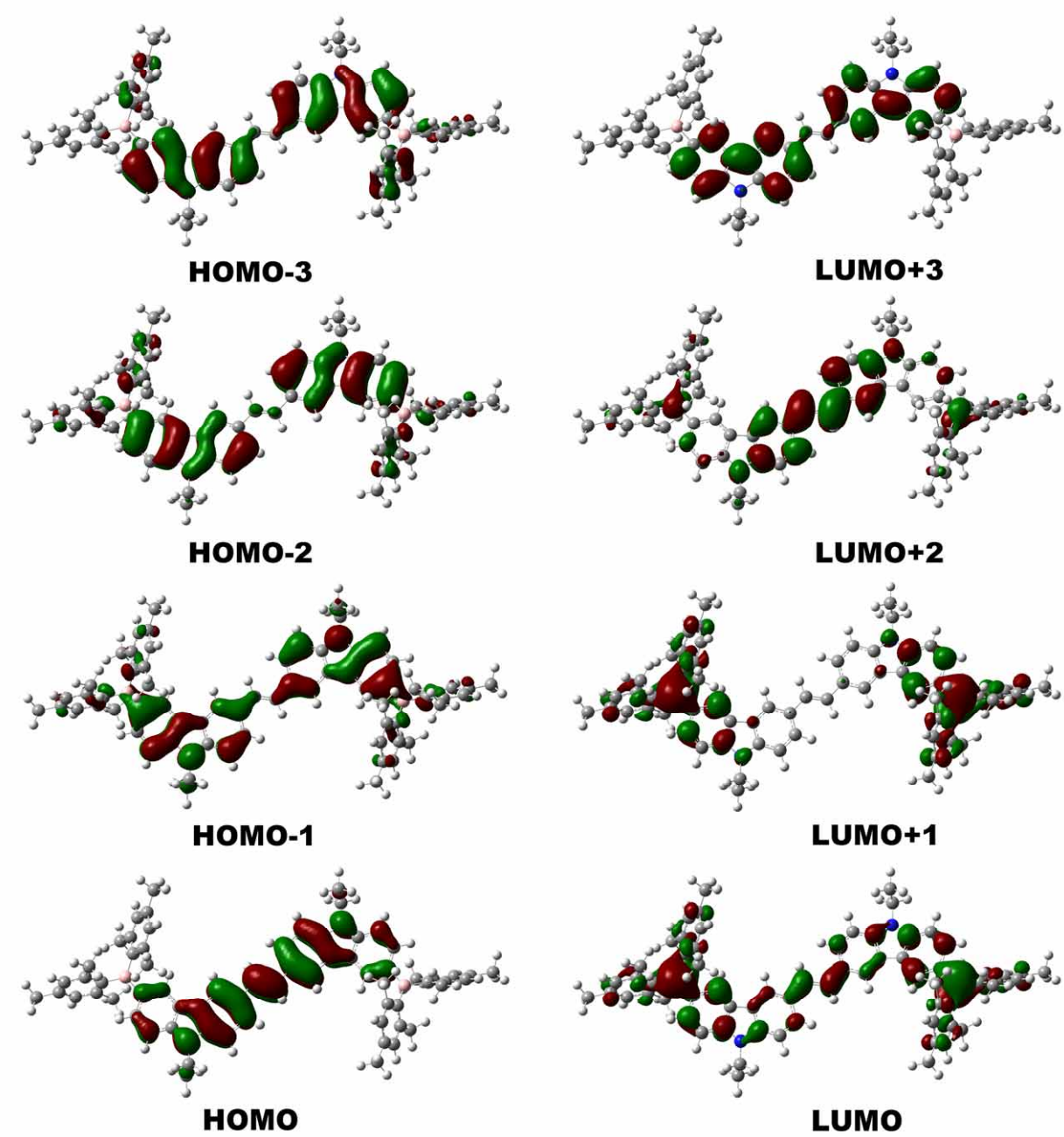

Fig. S1 Frontier orbitals of compound **BCCB**.

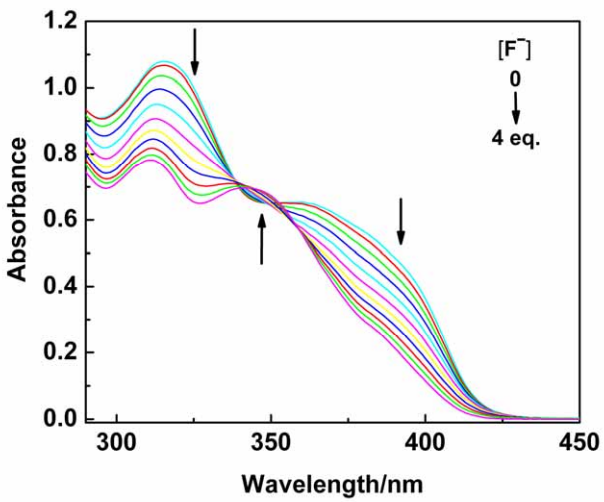

Fig. S2 Absorption spectra of **BCCB** (1.0×10^{-5} M) in DMSO upon stepwise addition of F^-.

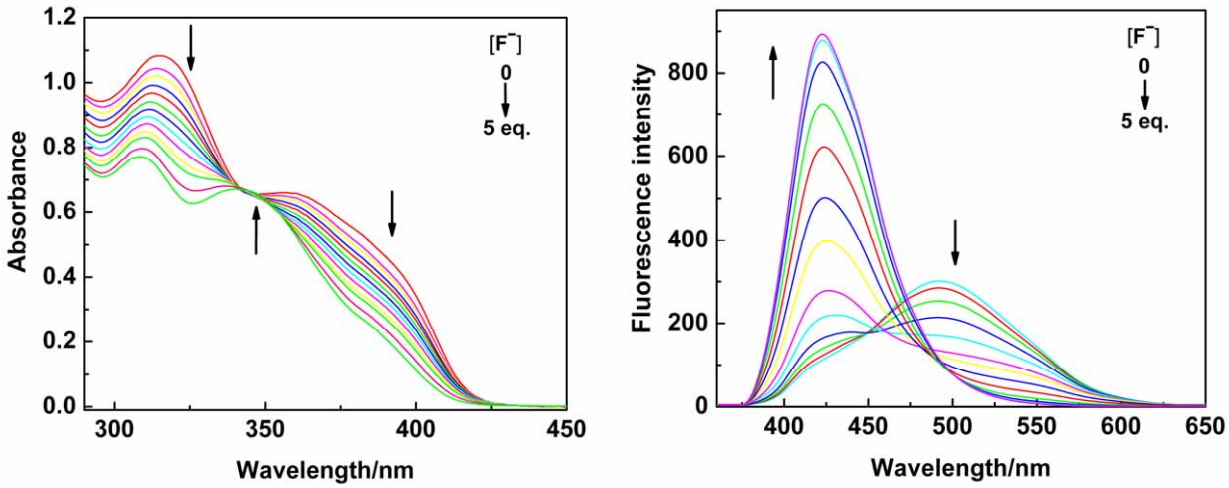

Fig. S3 Absorption and fluorescence spectra of **BCCB** (1.0×10^{-5} M) in DMSO upon stepwise addition of CN^-. Excited at 380 nm.

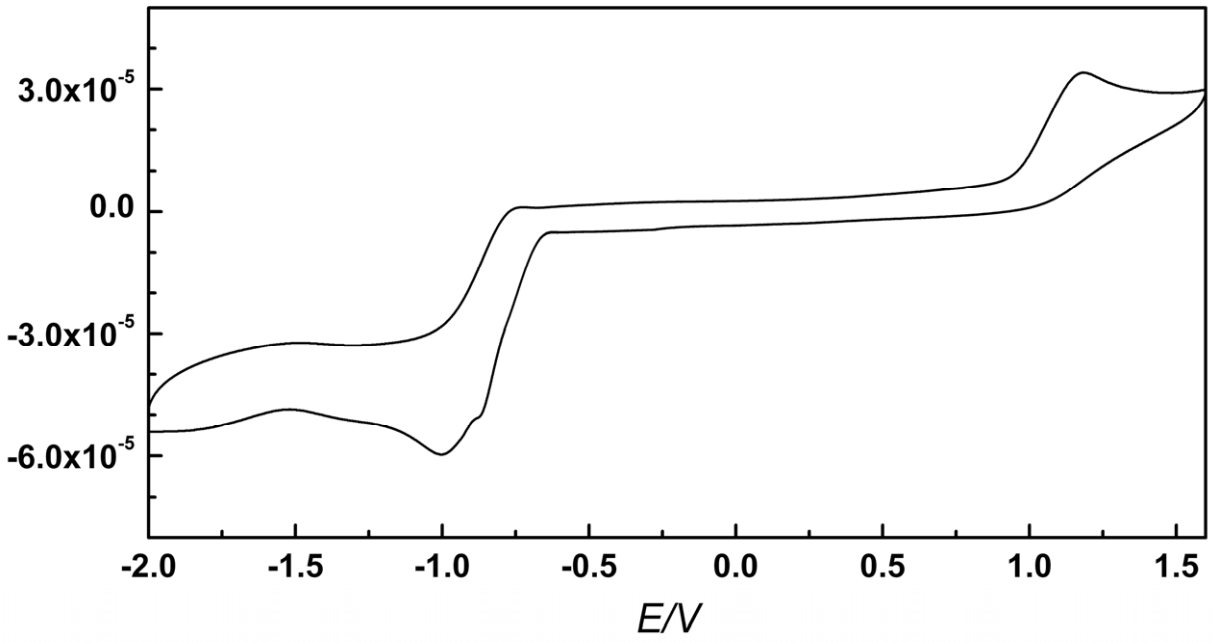

Fig. S4 Cyclic voltammogram of compound **BCCB** in MeCN at room temperature.

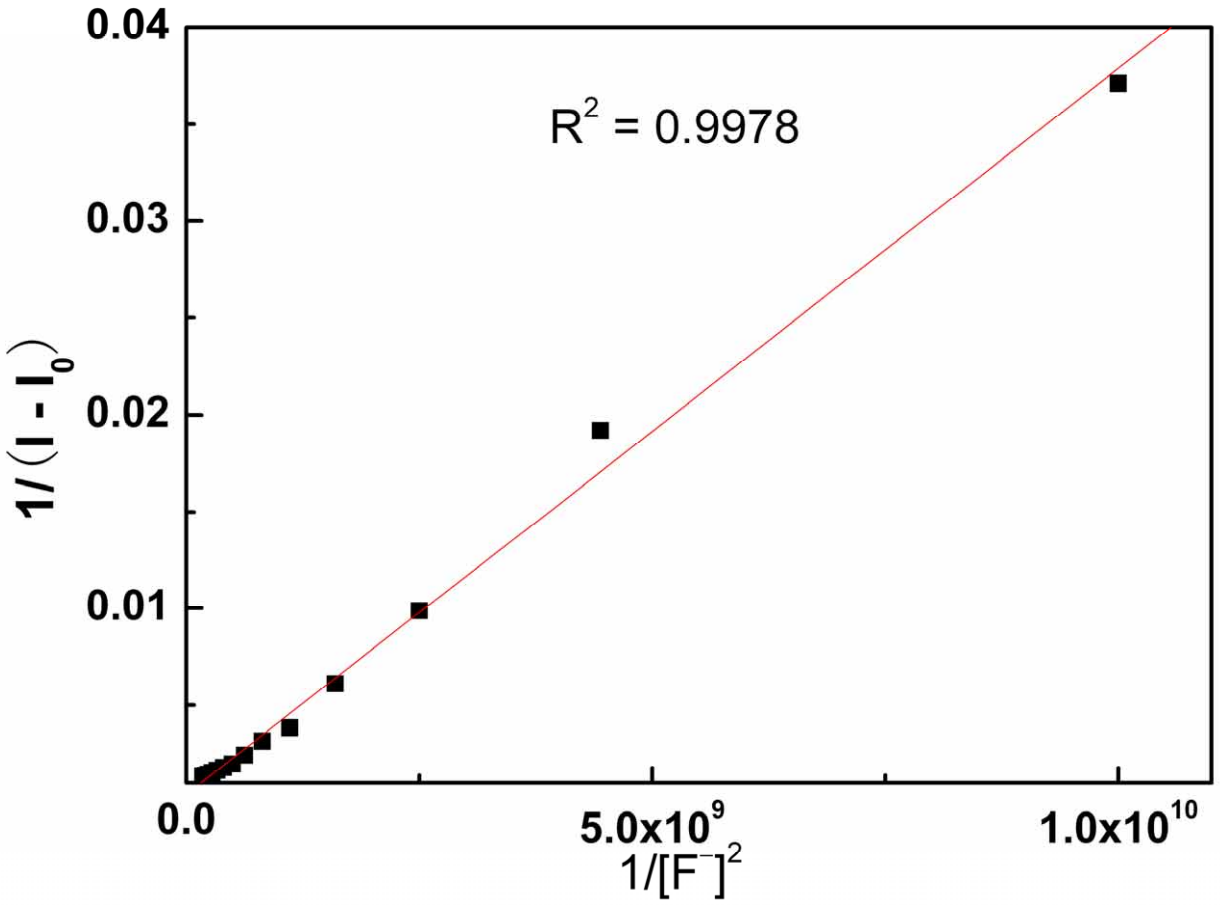

Fig. S5 1:2 Benesis-Hildebrand plot of compound **BCCB**.

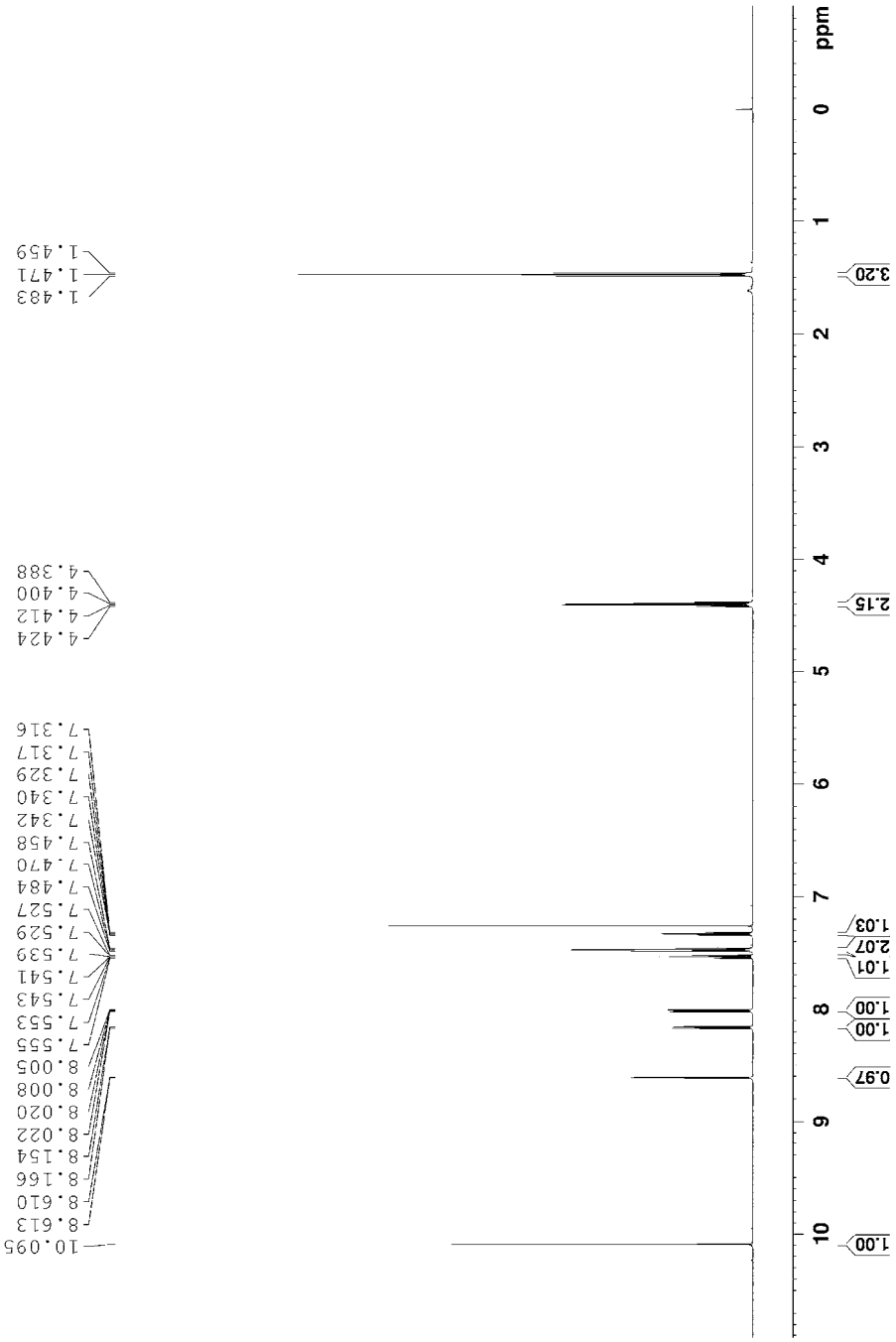

Fig. S6 ^{1}H NMR chart of compound **1** ($CDCl_3$).

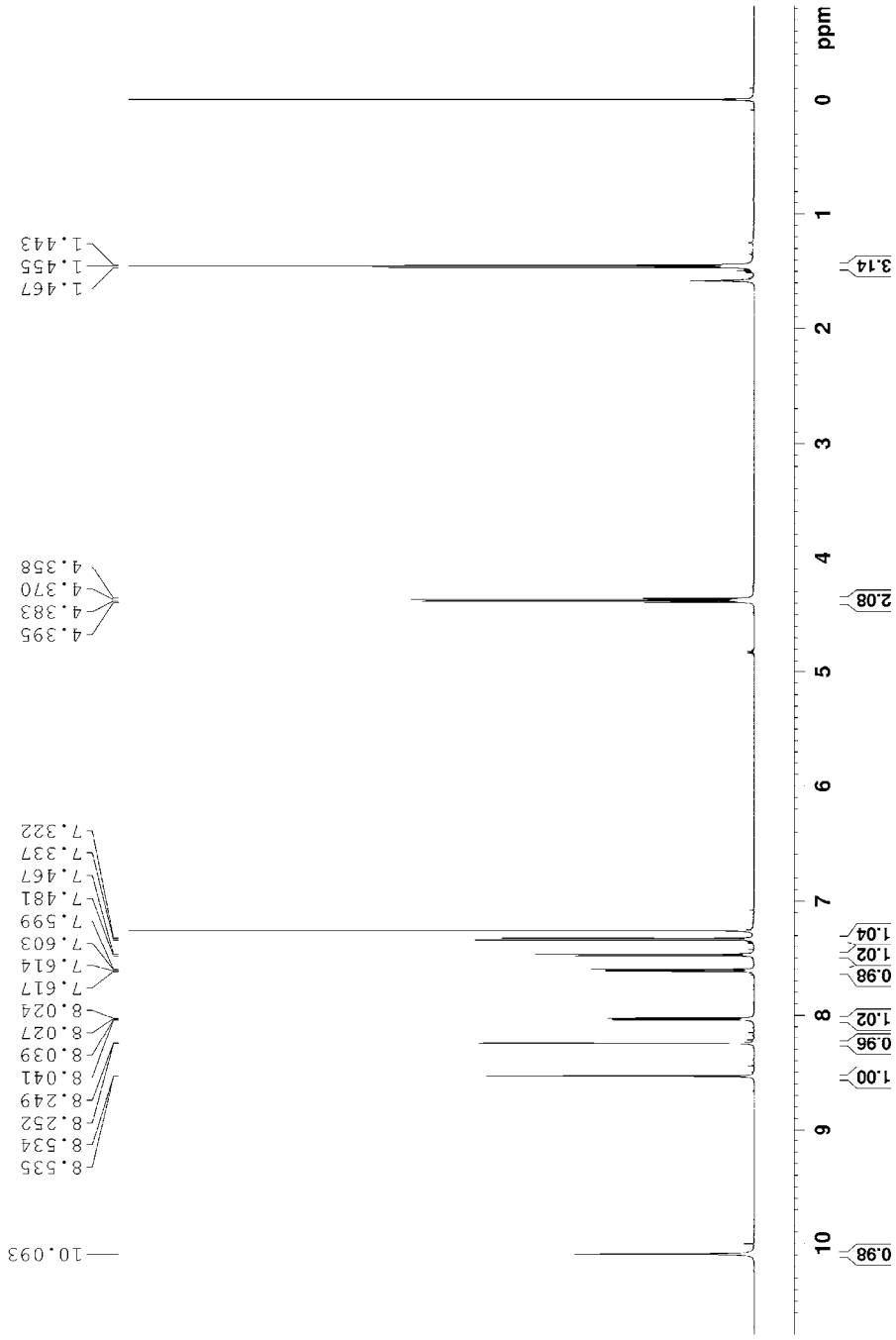

Fig. S7 ^{1}H NMR chart of compound **2** ($CDCl_3$).

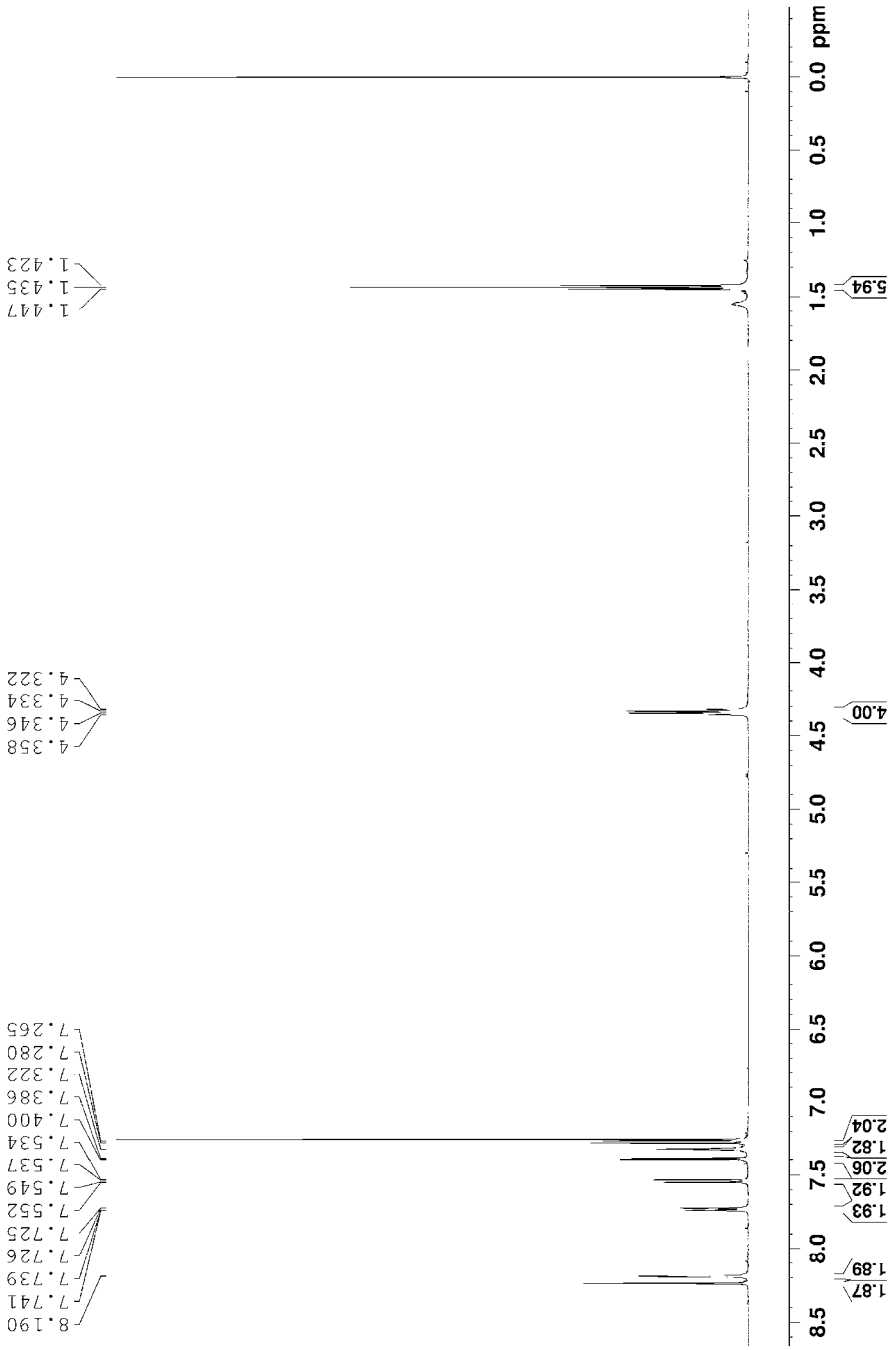

Fig. S8 ^{1}H NMR chart of compound **3** ($CDCl_3$).

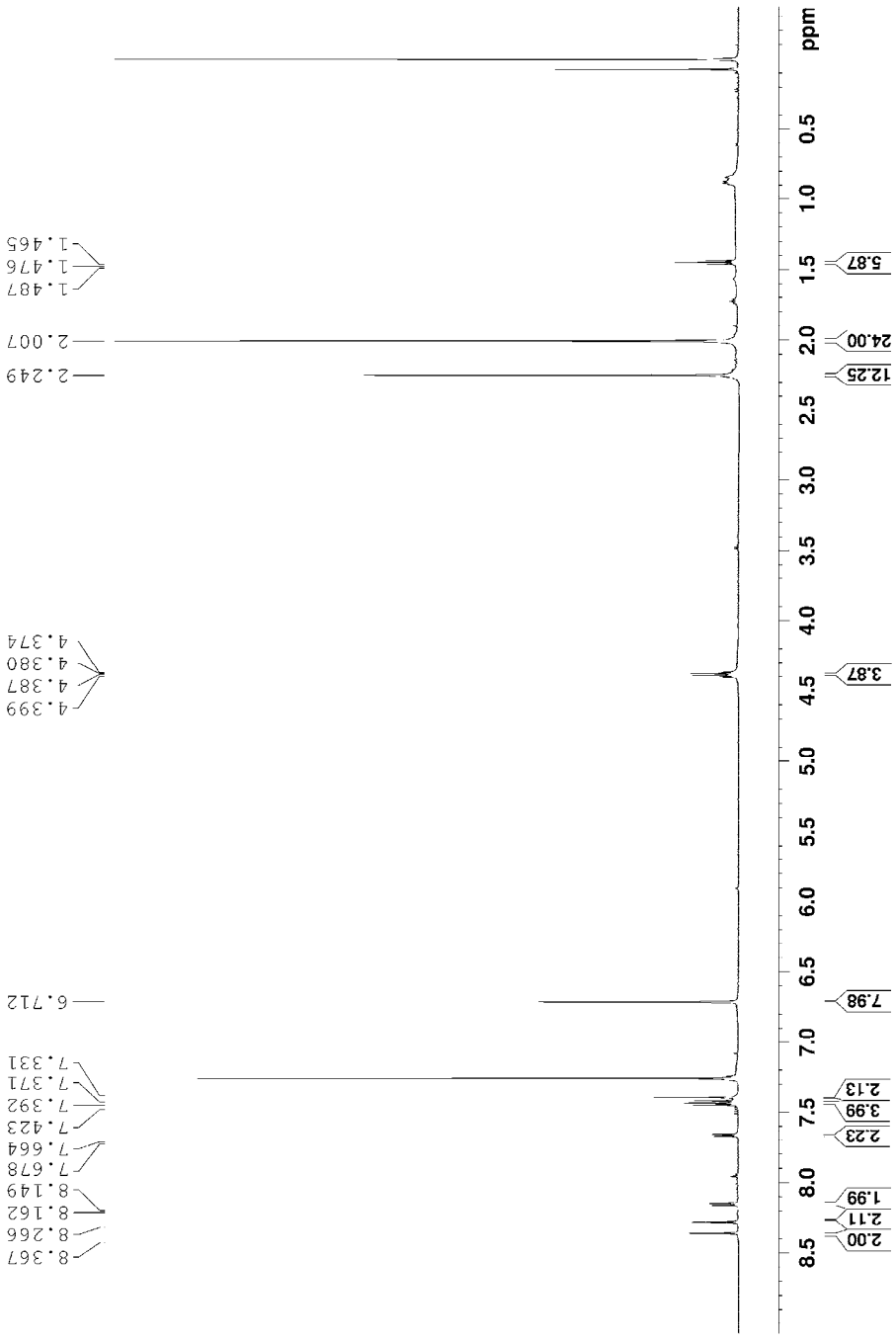

Fig. S9 ^{1}H NMR chart of compound **BCCB** ($CDCl_3$).

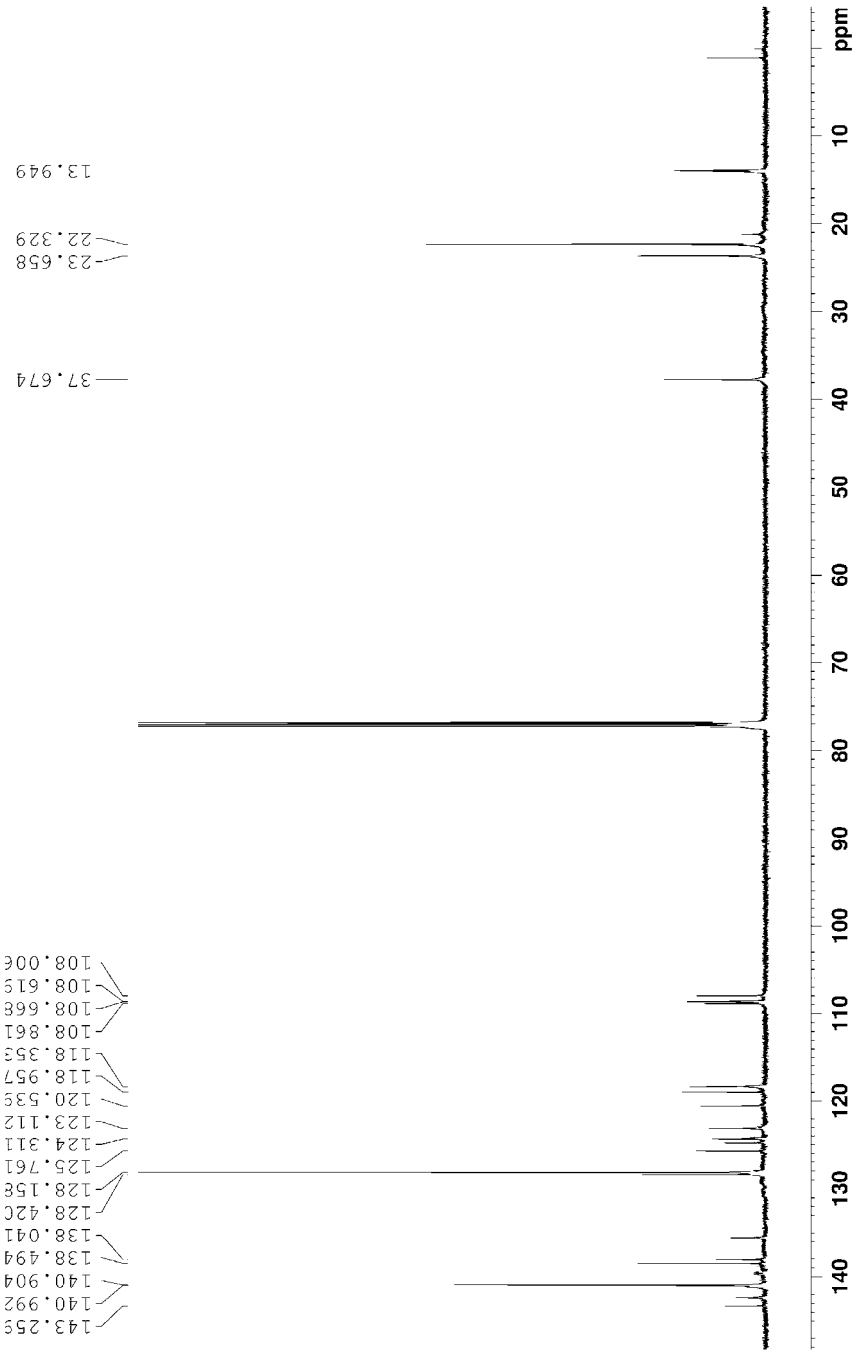

Fig. S10 ^{13}C NMR chart of compound **BCCB** ($CDCl_3$).