

Understanding the interaction mechanism of carbazole/anthracene with *N,N*-dimethylformamide: NMR study substantiate carbazole separation

Hui Cao,^{#ab} Mengyu Dou,^{#ab} Zexiang Lyu,^{#ab}, Yingxiong Wang,^{ab} Christian Marcus Pedersen^c and Yan Qiao^{*ab}

^a State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, 27 South Taoyuan Road, Taiyuan 030001, China

^b Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China

^c Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark

E-mail: qiaoy@sxicc.ac.cn

These authors contributed equally to this work.

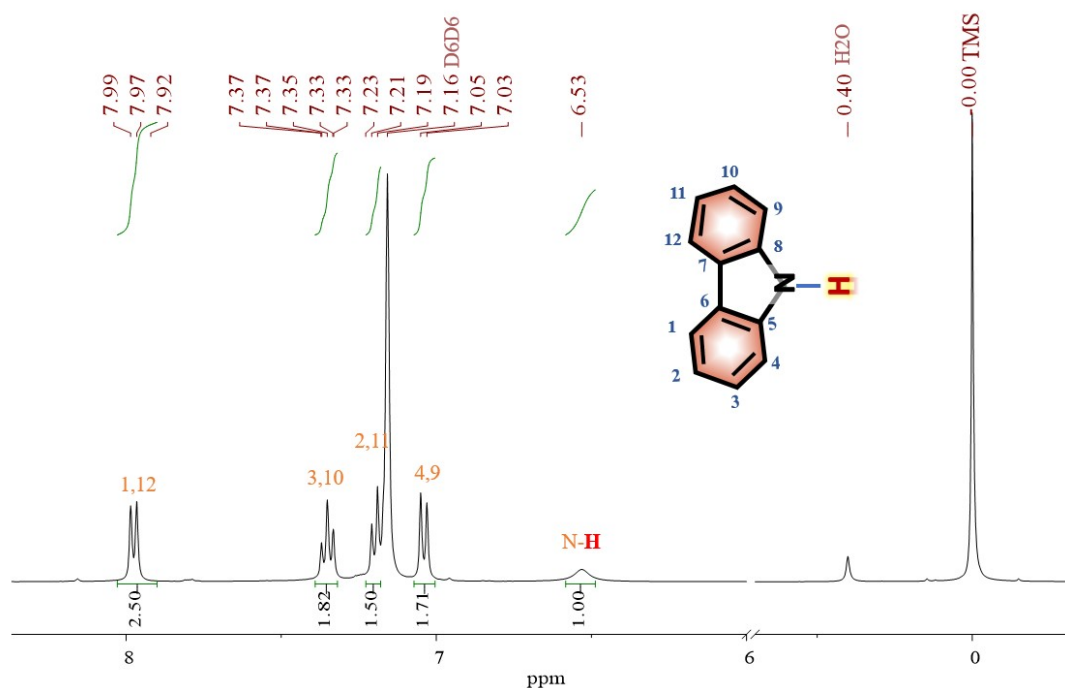


Fig. S1. The ¹H NMR spectrum of carbazole in C₆D₆ at 25 °C. The peak area ratio of carbazole from low field to high field is about 2:2:2:2:1, which is consistent with theoretical values.

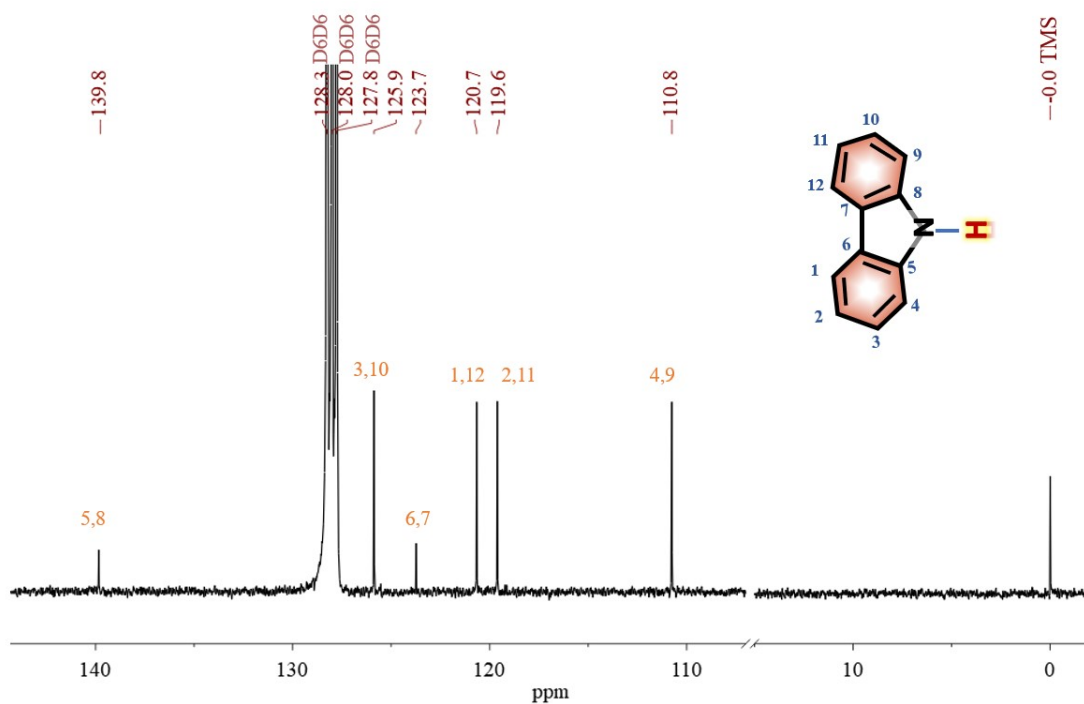


Fig. S2. The ^{13}C NMR spectrum of carbazole in C_6D_6 at 25°C .

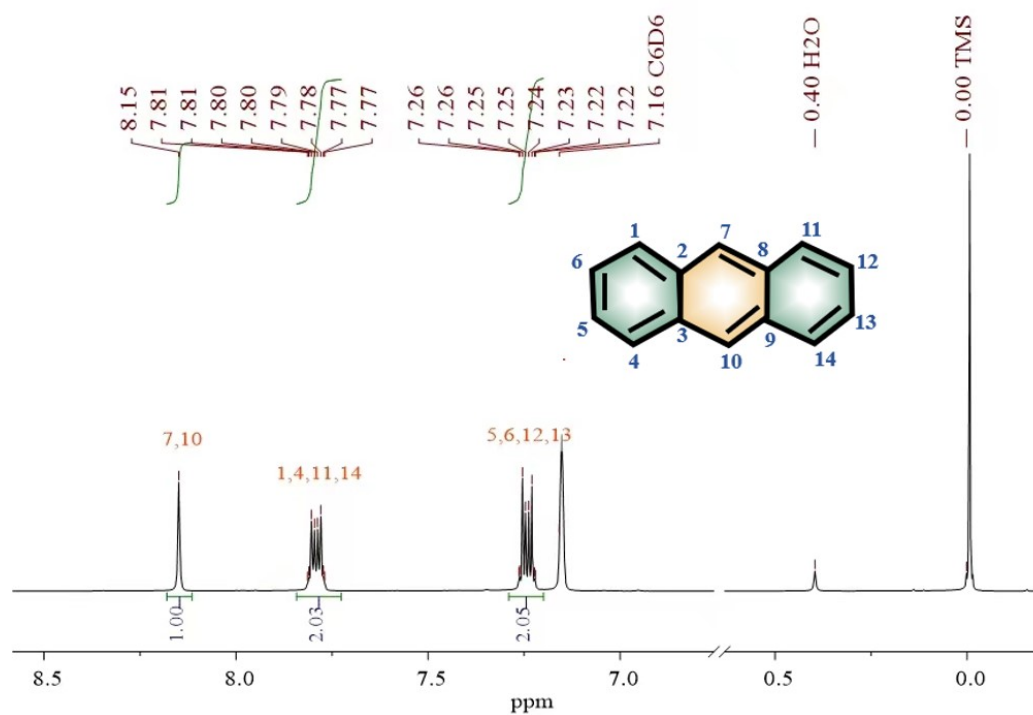


Fig. S3. The ^1H NMR spectrum of anthracene in C_6D_6 at 25°C . the peak area ratio of 1:2:2.

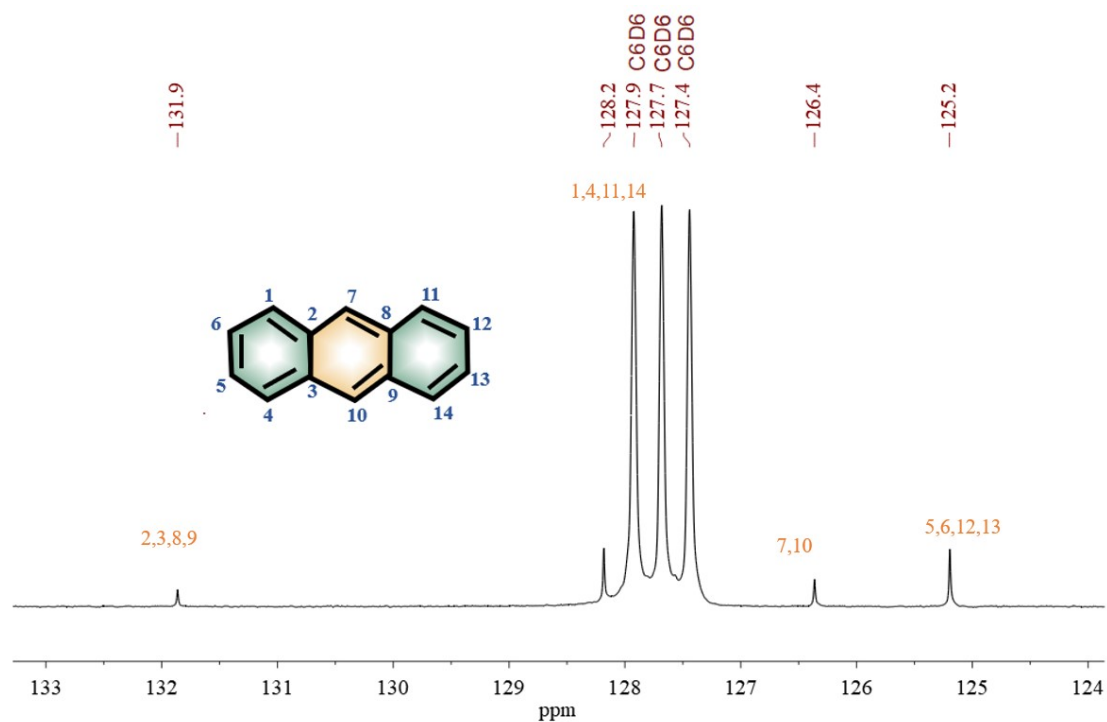


Fig. S4. The ^{13}C NMR spectrum of anthracene in C_6D_6 at 25°C .

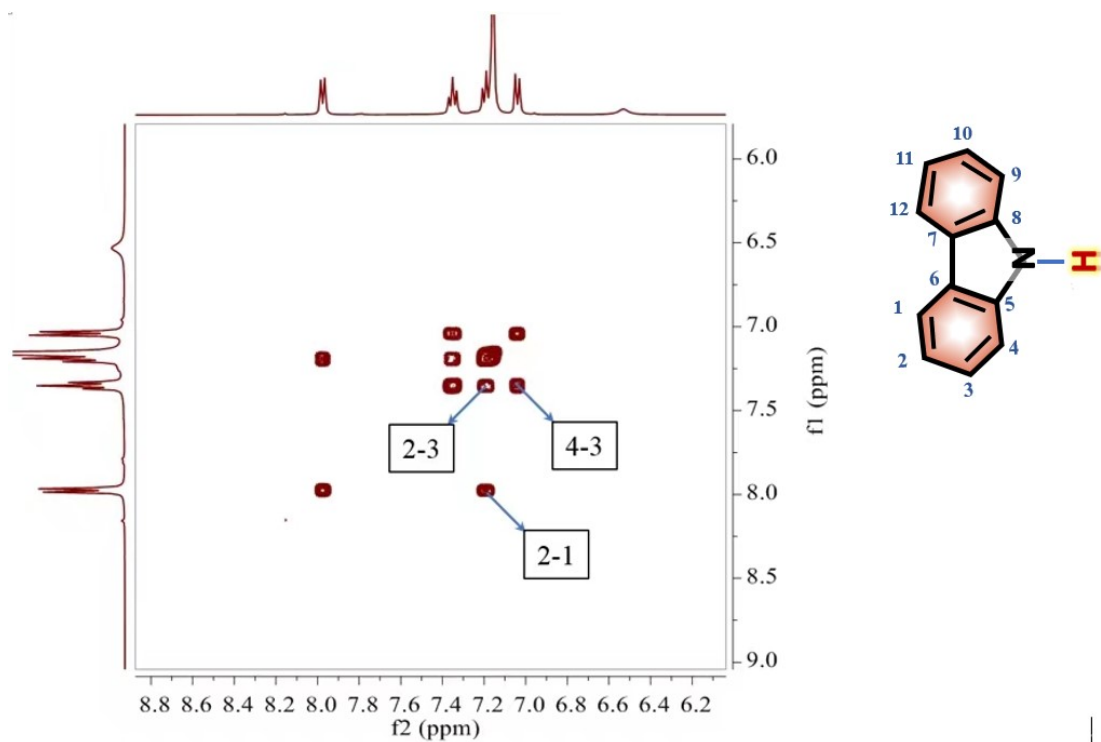


Fig. S5. The ^1H - ^1H COSY spectrum of carbazole in C_6D_6 at 25°C .

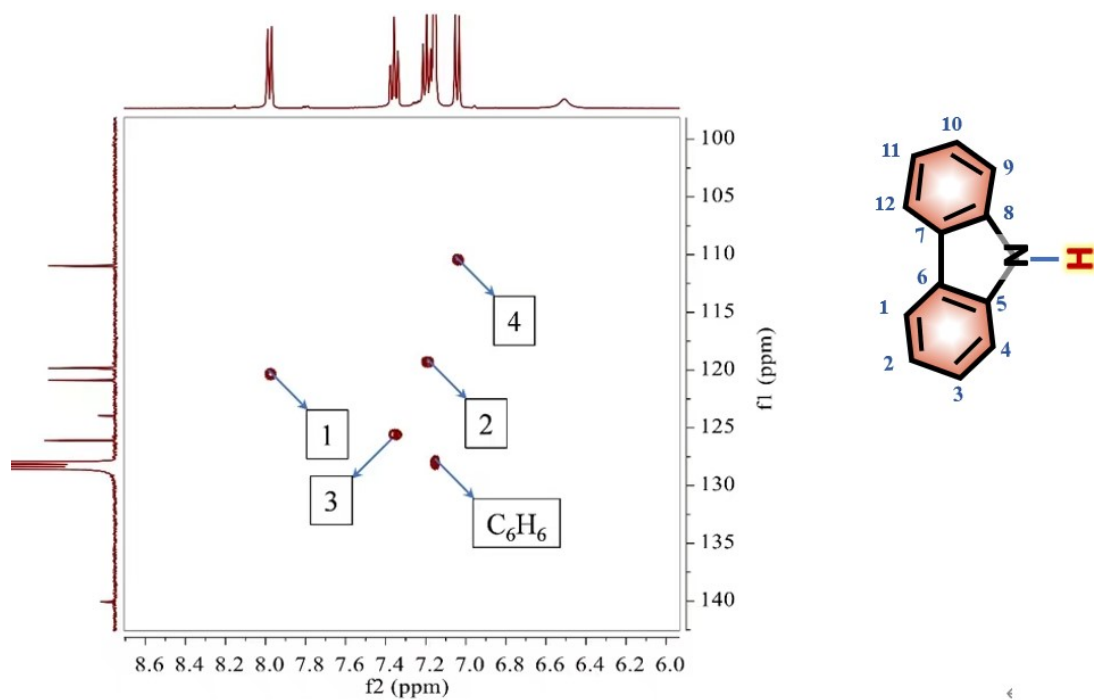


Fig. S6. The ^1H - ^{13}C HSQC spectrum of carbazole in C_6D_6 at 25 °C.

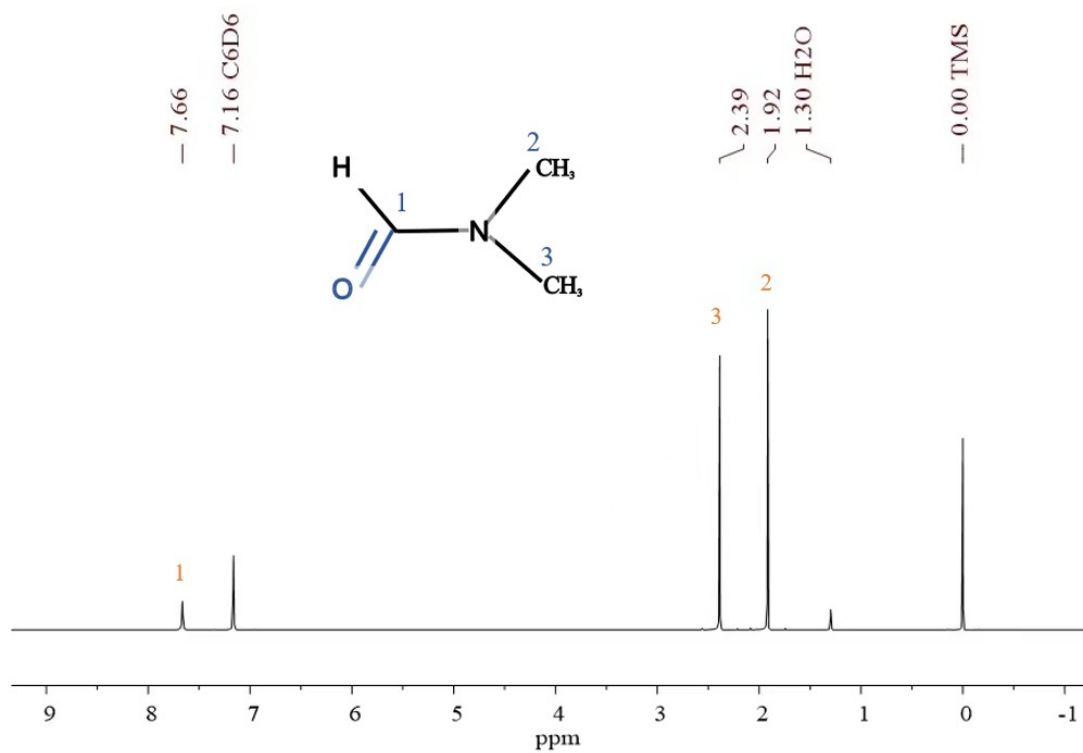


Fig. S7. The ^1H NMR spectrum of DMF in C_6D_6 at 25 °C.

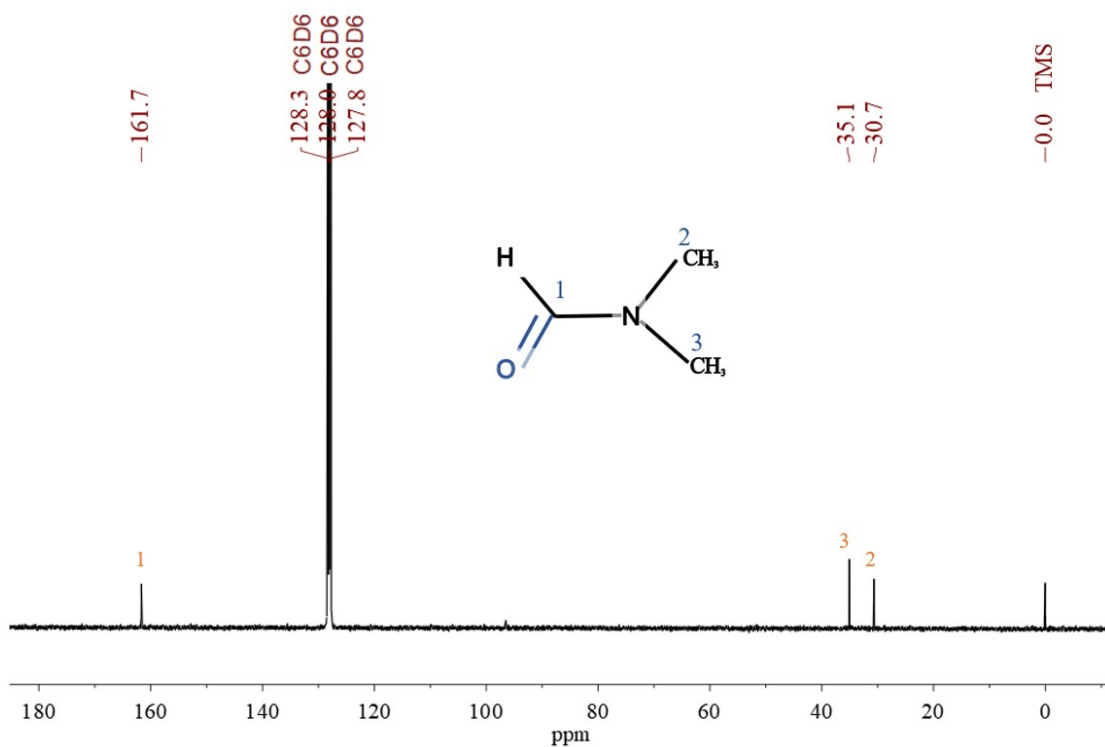


Fig. S8. The ^{13}C NMR spectrum of DMF in C_6D_6 at 25 °C.

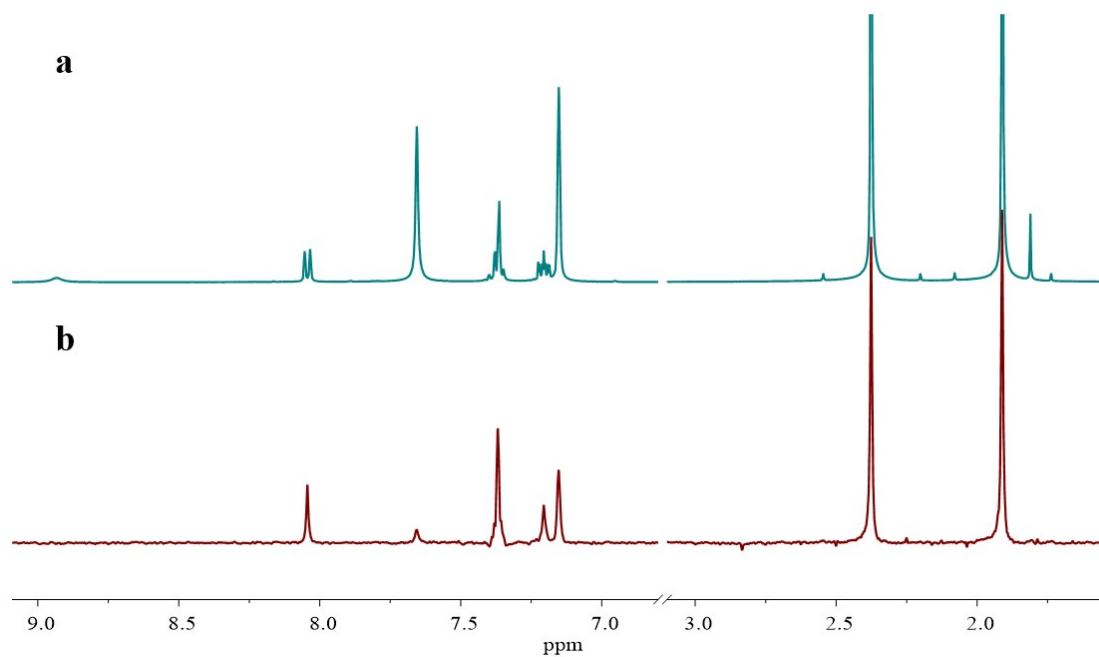


Fig. S9. The ^1H NMR spectra of 2.0 mg carbazole and 7.1 mg DMF in deuterated benzene and at 25 °C. (a) Conventional ^1H NMR spectrum, (b) Pure shift NMR spectrum.

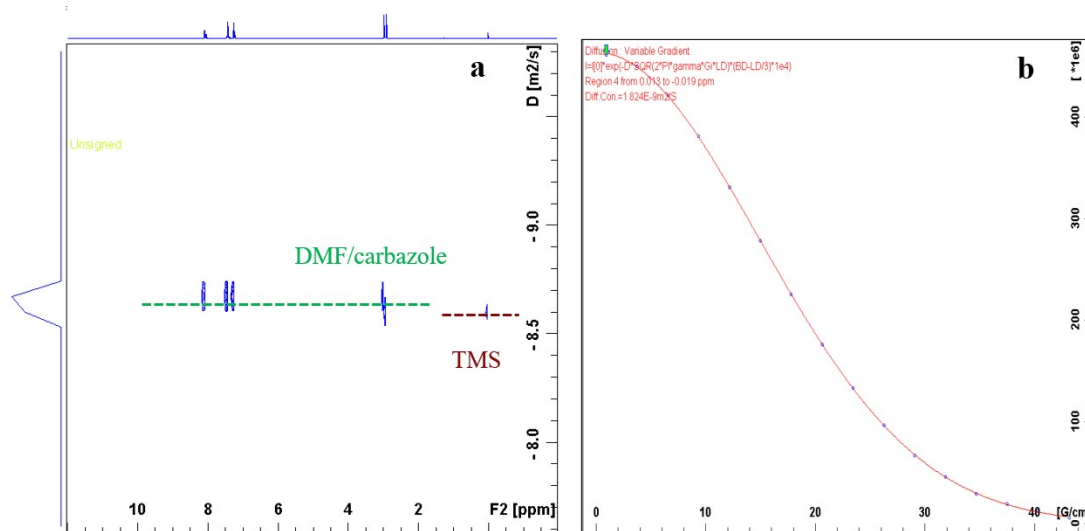


Fig. S10. The spectra of carbazole after adding DMF at 25 °C. (a) DOSY spectrum (b) Diffusion curve.

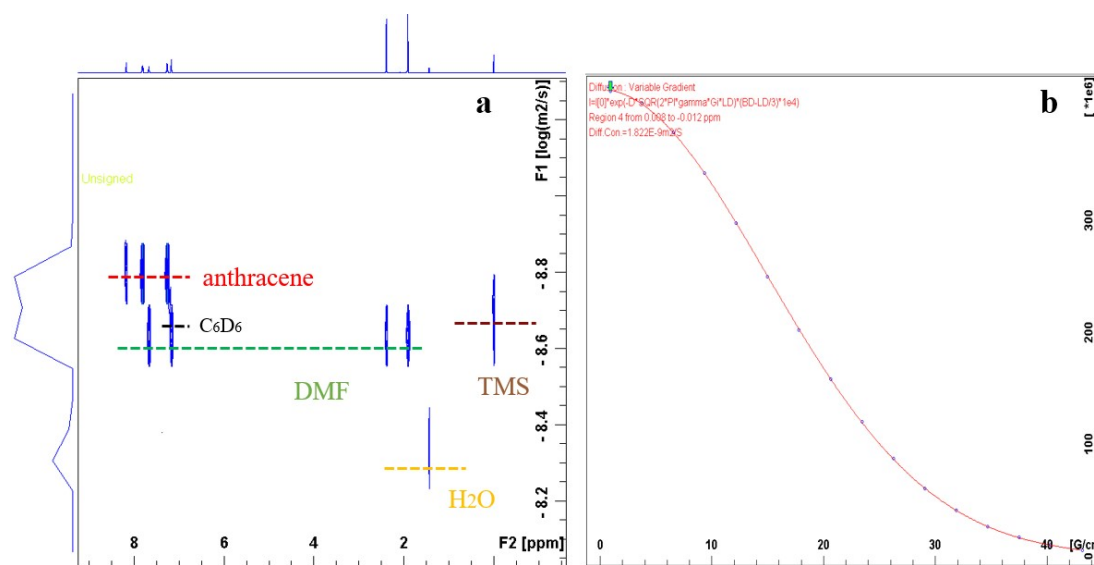


Fig. S11. The spectra of anthracene after adding DMF at 25 °C. (a) DOSY spectrum (b) Diffusion curve.