A Benzimidazol Functionalized NDI Derivative for Recyclable Fluorescent Detection Cyanide in Water

Qi Lin [a*], Lu Liu [a], Feng Zheng [a], Peng-Peng Mao [a], Juan Liu [b*], You-Ming Zhang [a], Hong Yao [a] and Tai-Bao Wei [a*]

[a] *Key Laboratory of Eco-Environment-Related Polymer Materials, Ministry of Education of China; Key Laboratory of Polymer Materials of Gansu Province; College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu, 730070. P. R. China*

[b] *College of Chemical Engineering, Northwest University for Nationalities, Lanzhou, 730000, P. R. China*

1. Experimental

1.1 Materials and instruments

All anions were used as the sodium salts while all cations were used as the perchlorate salts, which were purchased from Alfa Aesar and used as received. Other reagents used in the study were analytical grade. Fresh double distilled water was used throughout the experiment. All other reagents and solvents were commercially available at analytical grade and were used without further purification. ^{1}H NMR spectra were recorded on a Mercury−600BB spectrometer at 600 MHz and ^{13}C NMR spectra were recorded on a Mercury−600BB spectrometer at 150 MHz . Chemical shifts are reported in ppm downfield from tetramethylsilane (TMS, δ scale with solvent resonances as internal standards). Low-resolution mass spectra were recorded on a Bruker Esquire 6000 MS instrument. The infrared spectra were performed on a Digilab FTS-3000 Fourier transform-infrared spectrophotometer. Melting points were measured on an X-4 digital melting-point apparatus (uncorrected). Ultraviolet-visible (UV-vis) spectra were recorded on a Shimadzu UV-2550 spectrometer. Fluorescence spectra were recorded on a Shimadzu RF-5301PC spectrofluorophotometer.The infrared spectra were performed on a Digilab FTS–3000 FT–IR spectrophotometer.

1.2 General procedure for fluorescence experiments

Fluorescence spectroscopy was carried out keeping the host concentration constant in ethanol solution on a Shimadzu RF-5301PC spectrofluorophotometer.

1.3. General procedure for fluorescence spectra experiments

*Corresponding author. Tel.: +86 931 7973120.
E-mail address: linqi2004@126.com, liujuan656@126.com; weitaibao@126.com.

All fluorescence spectra were recorded on a Shimadzu RF-5301fluorescence spectrometer after the addition of tetrabutylammoniumsalts and in water, while keeping the ligand concentrationconstant (2.0×10^{-5} M). The excitation wavelength was 455 nm. Solutions of anions were prepared from the NaCN andtetrabutylammonium salts of F^-, Cl^-, Br^-, I^-, AcO^-, $H_2PO_4^-$,HSO_4^-, ClO_4^- and SCN^-.

1.4 General procedure for ^{1}H NMR titrations

For ^{1}H NMR titrations, three stock solutions were prepared: one of them contained the host only in DMSO-d_6, the second one contained an appropriate concentration of guest in DMSO-d_6. The third one contained an appropriate concentration of host and guest in DMSO-d_6. Aliquots of the two solutions were mixed directly in NMR tubes.

1.5 General procedure for concentration-dependent ^{1}H NMR measurements

The concentration-dependent 1H NMR was carried out by gradually increasing the concentration of the DMSO-d_6 solution of **L2**. The initial concentration of the **L2** is 1.0 mM, the concentration was adjusted by directly addition right amount of powdery **L2** into the DMSO-d_6 solution.

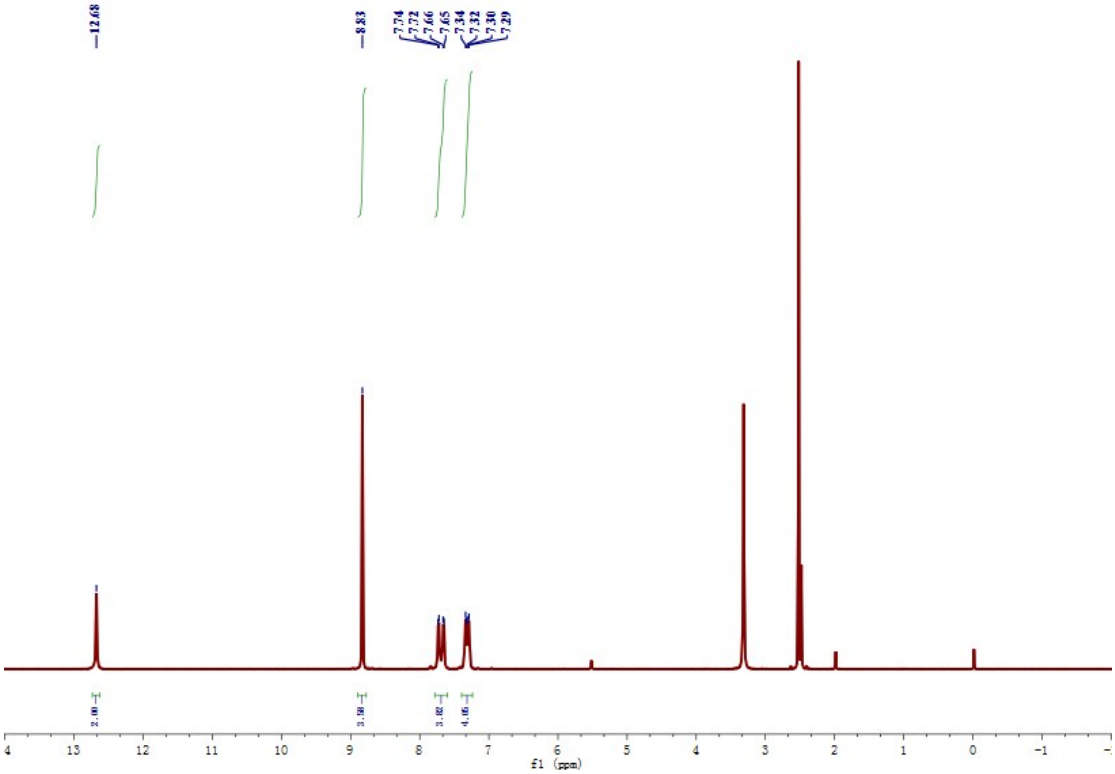

Fig. S1 ^{1}H NMR spectra of compound **L2** in DMSO-d_6.

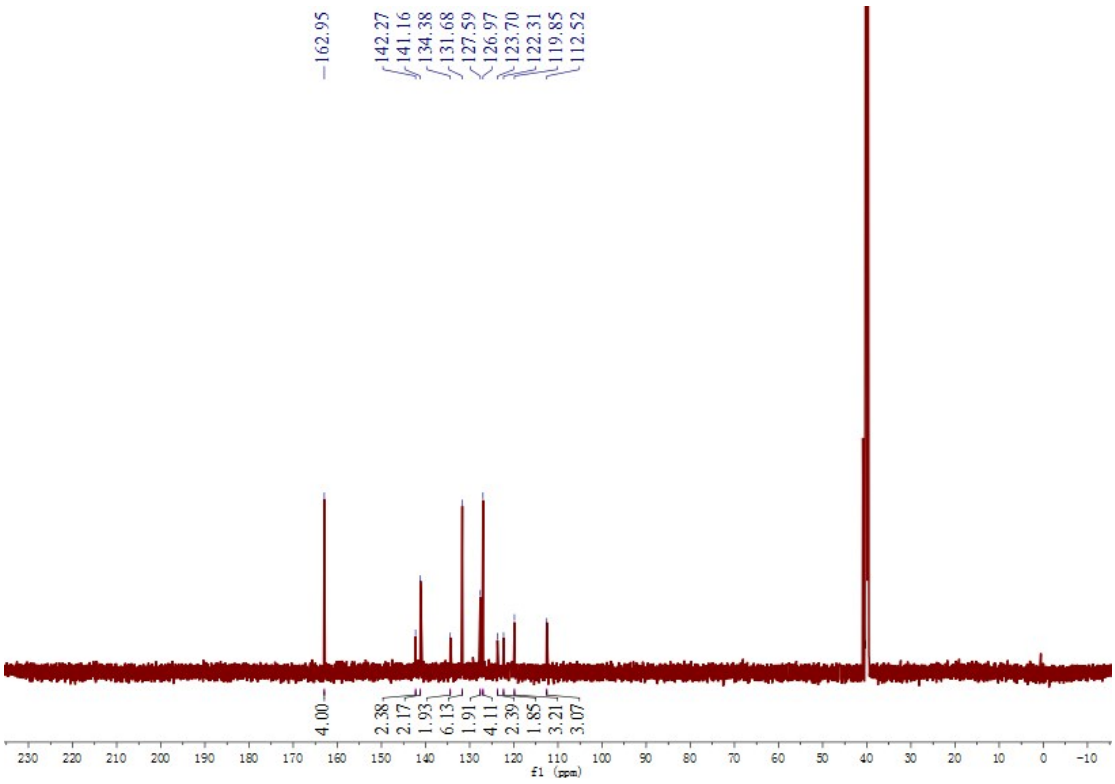

Fig. S2 ^{13}C NMR spectra of compound **L2** in DMSO-d_6.

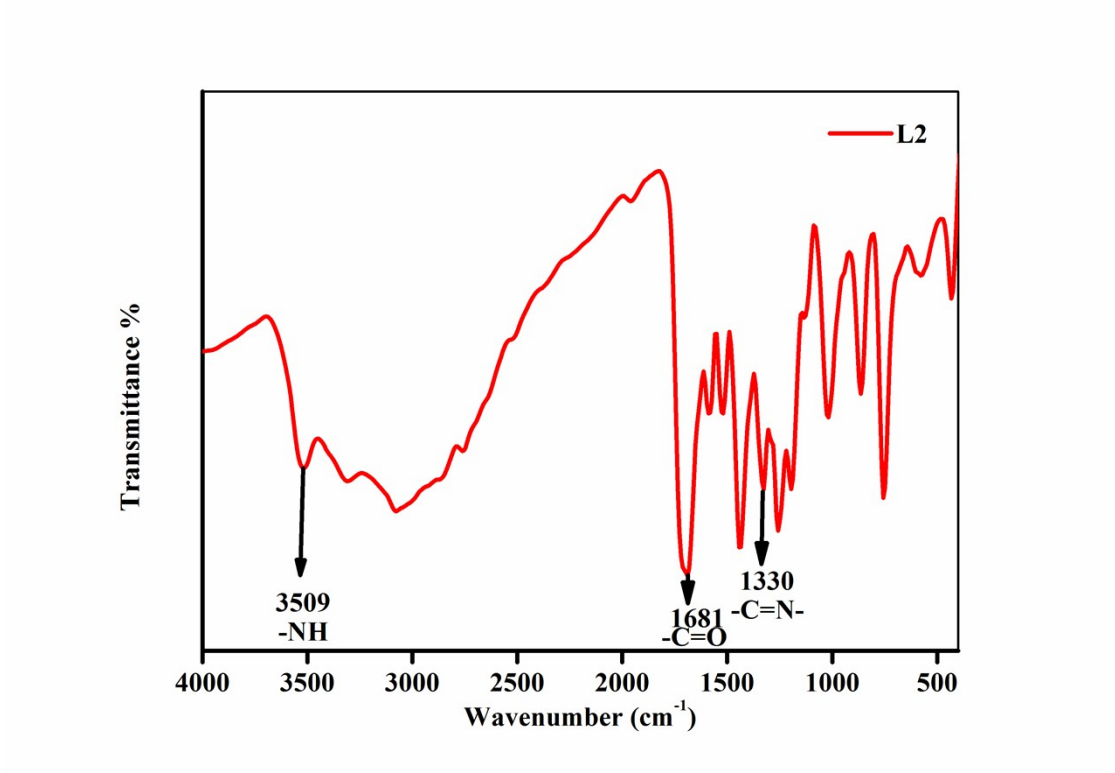

Fig. S3 IR spectra of sensor L2 in KBr disks.

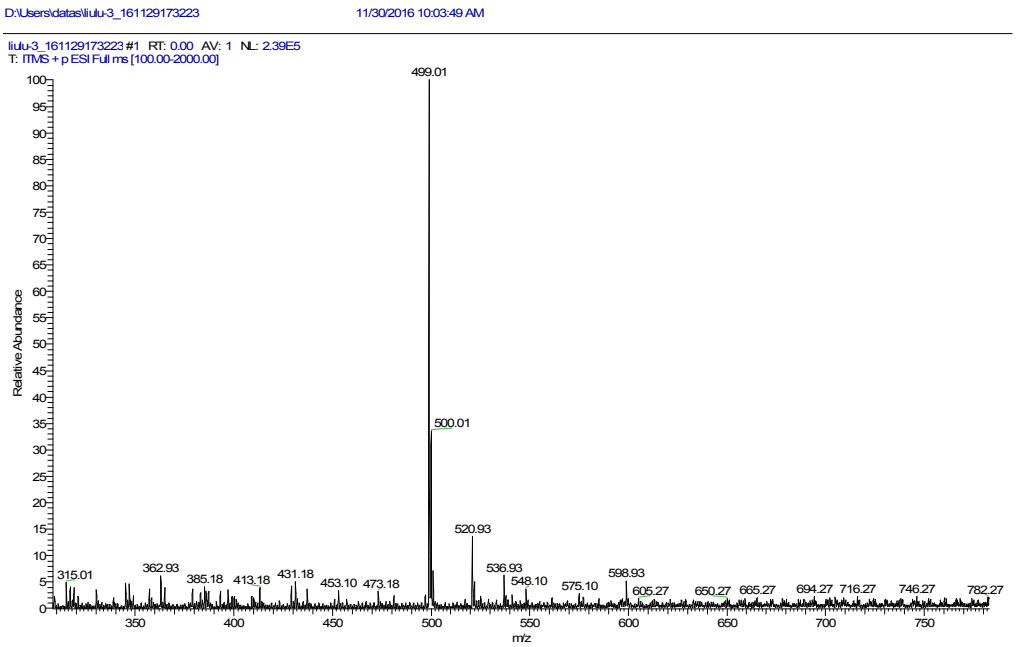

Fig. S4 Electrospray ionization mass spectrum of **L2**.

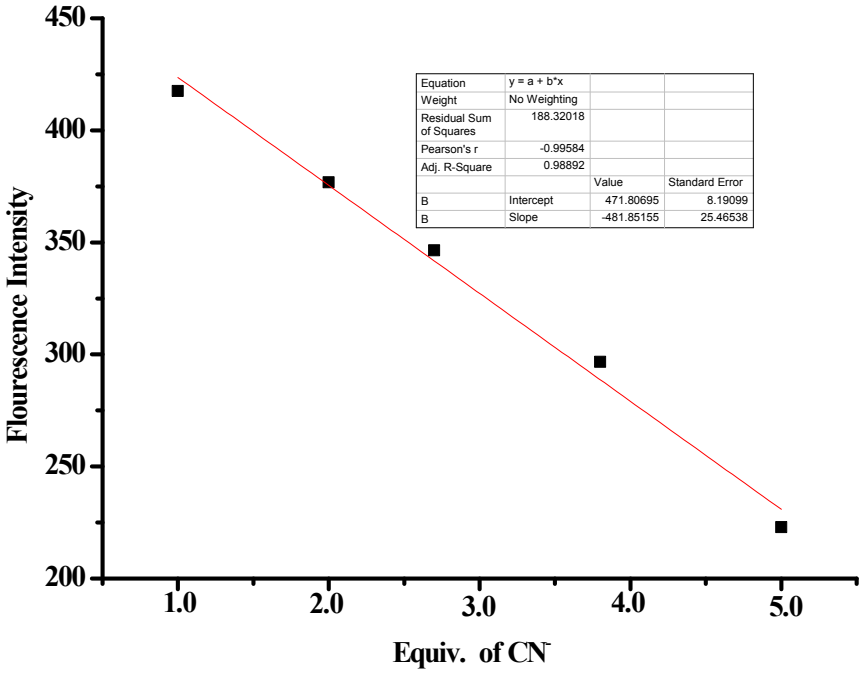

Fig. S5 The photograph of the linear range.

Linear Equation: Y= -481.851X+471.80

R^2=0.99584 S=4.851×10^8

$$\delta = \sqrt{\frac{\Sigma(Fi - F0)^2}{N - 1}} = 142.652 \text{ (N=20)}$$

LOD =K × δ/S = 8.82 ×10^{-7} M

K=3

F_0 is the fluorescence intensity of **L2**, F_1 is the average of the F_0.

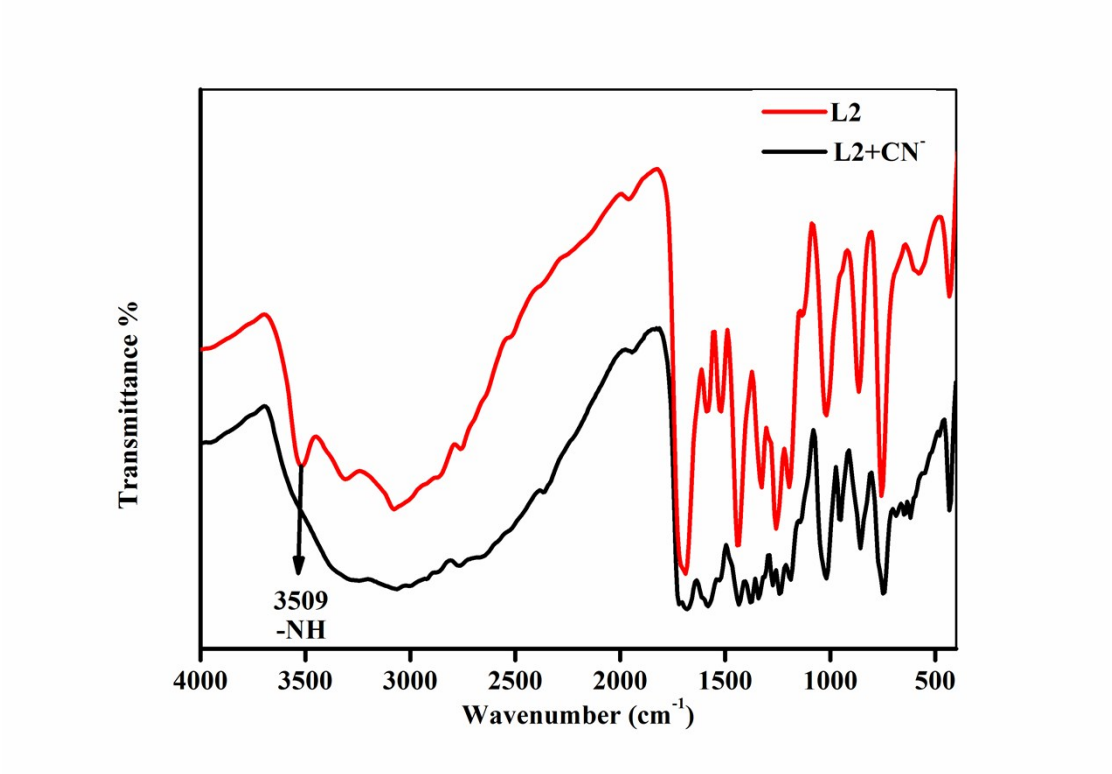

Fig. S6. Infrared spectra of **L2** (black line) and its complex (red line).