Amidine-based Fluorescent Chemosensor with High Applicability for Detection of CO_2: A Facile Way to "See" CO_2

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Supporting Information

Materials and Methods

DBU(1,8-diazabicyclo-[5,4,0]-undec-7-ene), TPE (tetraphenylethene) and 5-Amino-1-pentanol were purchased from Alfa Aesar and used as received. Isopropanol was purchased from Beijing chemical works. CO_2 gas was 99.999%.

^{1}H-NMR spectra were measured on a Bruker minispec spectrometer in $CDCl_3$. FT-IR spectra were taken on an AVATAR FT-IR spectrophotometer. PL spectra were recorded on a RF5301-PC spectra fluorometer. Dynamic viscosity was measured on a Brookfield LVDV-III U at room temperature. Particle sizes of the TPE nano-aggregates in the IL mixtures were determined at room temperature by Dynamic Light Scattering using a CORDOUAN VASCO（CORDOUAN Technologies）. In a typical run, an 1.2 mL of TPE-contained mixture with TPE concentration of 3.3 mg/mL was used. CO_2 gas was bubbled into the solution through a PTFE tube with diameter of 0.5 mm. The bubbling rate was controlled by a pressure regulator made by Brooks Instrument and fixed at 4 mL/s.

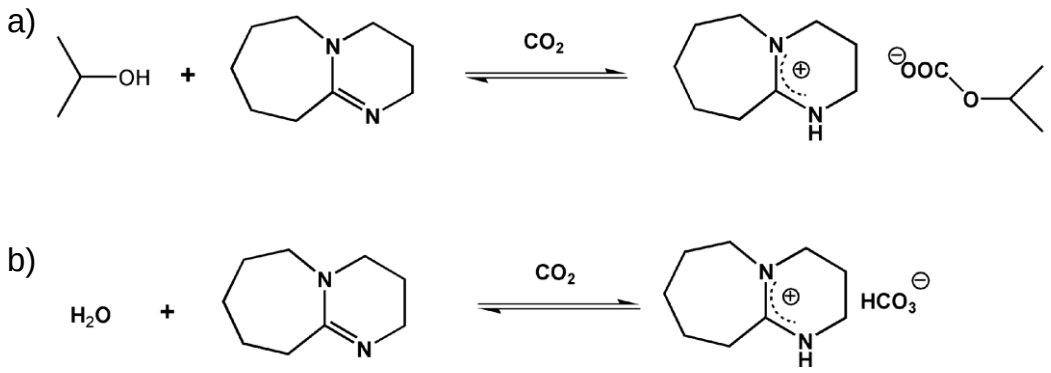
Table S1:

Table S1. The chemosensor systems with specific volume ratios of DBU to APN studied in our work

volume ratio of DBU to APN (v:v)	Volume（mL）		Mole (mmol)	
	DBU	APN	DBU	APN
1:1	0.6	0.6	4.0	5.5
2:1	0.8	0.4	5.3	3.7
3:1	0.9	0.3	6.0	2.7

Scheme S1:

Scheme S1. (a) The scheme of reaction of DBU with isopropanol when bubbled with CO_2. (b) The scheme of reaction of DBU with water when bubbled with CO_2.



Video S1:

An about 3-minute length of video file was provided: An Easy Way to “See” CO2_video.avi

Figure S1:

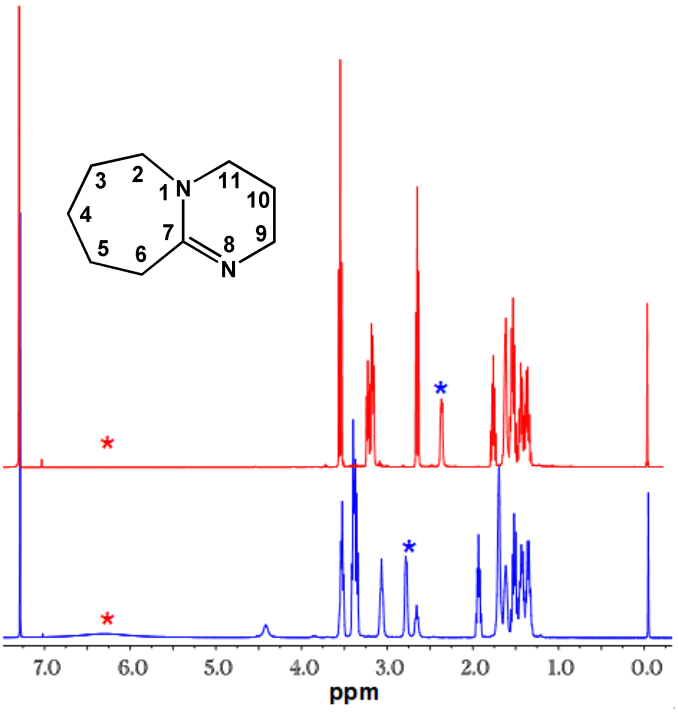


Figure S1. ^{1}H-NMR spectra of mixture of DBU and APN(1:1,v:v) in chloroform-*d* before(red) and after(blue) bubbled with CO_2. The red star shows the chemical shifts of proton of carboxylic groups formed after bubbled with CO_2. The blue star shows the signals of protons of C_6 downfield shifted from 2.34 ppm (before bubbled with CO_2) to 2.77 ppm after bubbled with CO_2.[1] Inset: Numbering scheme for positions in the DBU structure.

Figure S2:

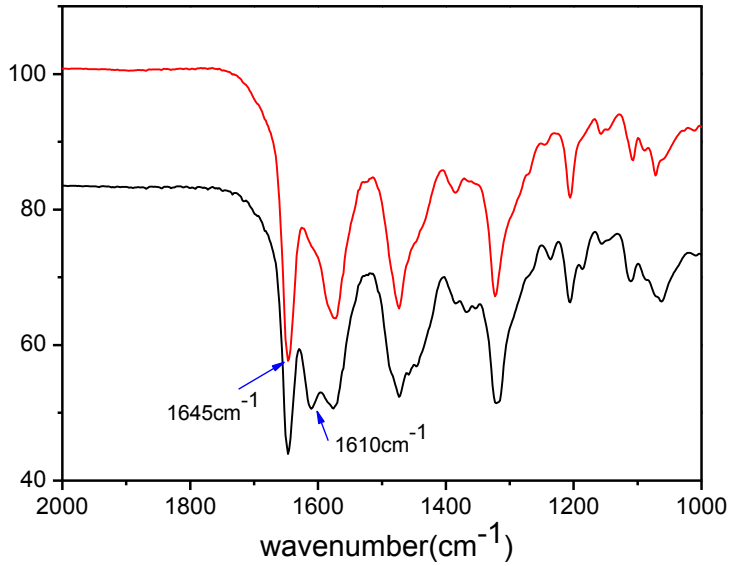


Figure S2. FT-IR spectra of mixture of DBU and APN (1:1,v:v) in chloroform-*d* before(black) and after(red) bubbled with CO_2. It was shown that a characteristic peak standing for the streching viberations of C=N on DBU shifted from 1610 cm^{-1} to 1645 cm^{-1} after bubbled with CO_2. [2]

Figure S3:

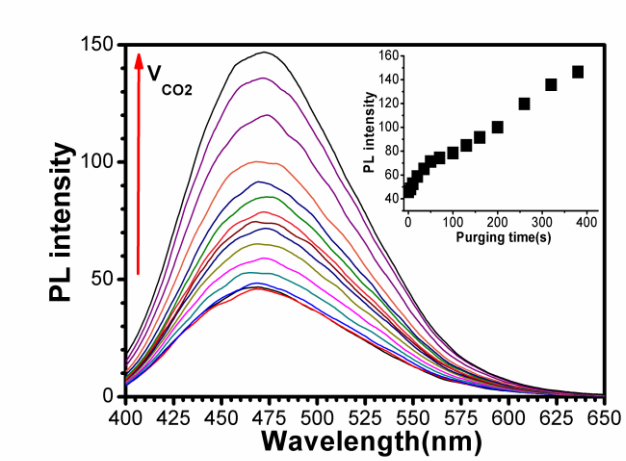


Figure S3. PL spectra of the TPE-contained (3.3mg) mixture (1.2mL) composited of DBU and APN (2:1,v:v) when bubbled with different volumes of CO_2.

Figure S4:

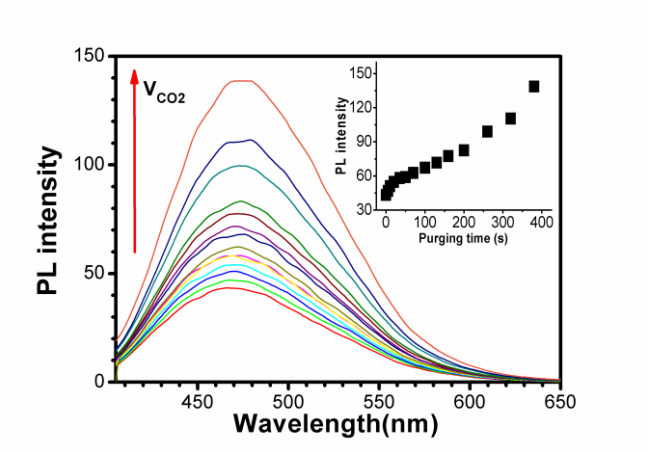


Figure S4. PL spectra of the TPE-contained (3.3mg) mixture (1.2mL) composited of DBU and APN (3:1,v:v) when bubbled with different volumes of CO_2.

Figure S5:

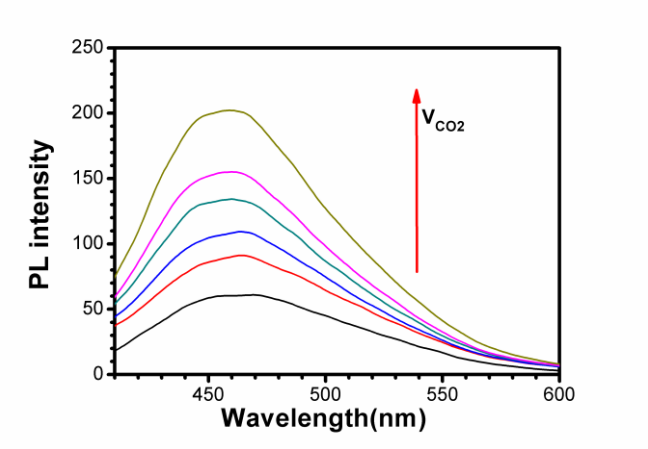


Figure S5. PL spectra of TPE-contained (3.3mg) mixture (1.2mL) composited of DBU and isopropanol (1:1,v:v) bubbled with different volumes of CO_2.

References

[1] Jessop, P. G.; Heldebrant, D. J.; Li, X.; Eckert, C. A.; Liotta, C. L. *Nature*. **2005**, 436, 1102-1102.
[2] Heldebrant, D. J.; Jessop, P. G.; Thomas, C. A.; Eckert, C. A.; Liotta, C. L. *J. Org. Chem*. **2005**,70, 5335-5338.