Supplementary Information

Sensitive Colorimetric Sensors for Visual Detection of Carbon Dioxide and Sulfur Dioxide

Chandrani Chatterjee and Ayusman Sen^{*} Department of Chemistry, Pennsylvania State University, University Park, PA 16802 (U.S.A.). E-mail: <u>asen@psu.edu</u>



Figure S1. Visual detection and estimation of the amount of dry CO₂ present within an enclosed atmosphere using a) Al_2O_3 -dimethylethanolamine-cresol red, b) Al_2O_3 -methyldiethanol amine-cresol red, and c) Al_2O_3 -triethanolamine-cresol red sensors. The visual color changes in response to 500 ppm, 800 ppm, 1600 ppm and 2600 ppm dry CO₂ in nitrogen are compared with a reference sensor left under ambient air (~ 400 ppm CO₂).



Figure S2. ¹³C NMR spectra of N,N-diisopropylethylamine in dry CDCl₃ in the presence of ¹³CO₂ (free CO₂, 124.4 ppm). The formation of bicarbonate was not observed.



Figure S3. ¹³C NMR spectra of N,N-diisopropylethylamine in CDCl₃ containing 20 μ L D₂O, in the presence of ¹³CO₂ (free CO₂, 124.4 ppm). The *in situ* formed bicarbonate peak is observed ~ 160.3 ppm.



Figure S4. ¹³C NMR spectra of ¹³CO₂ (free CO₂, 124.4 ppm) binding by MDEA, in the presence of 20 μ L D₂O, in CDCl₃. The resonance due to alkylcarbonate formation is observed ~159 ppm and the bicarbonate peak is observed ~161 ppm.



Figure S5. ¹³C NMR spectra of ¹³CO₂ (free CO₂, 124.4 ppm) binding by MDEA in dry CDCl₃. Only the *in situ* formed alkylcarbonate peak was observed ~ 159 ppm.



Figure S6. The ¹H NMR spectra of N-methyldiethanolamine in CDCl₃: a) before CO₂ uptake, b) after CO₂ uptake, and c) after CO₂ uptake in the presence of 20 μ L D₂O. New resonances appear only upon the uptake of CO₂ in the presence of water (Figure S6c).



Figure S7. ¹H NMR spectra of a) MDEA and b) SO₂ binding by MDEA in DMSO-d₆.



Figure S8. ¹³C NMR spectra of a) MDEA and b) SO₂ binding by MDEA in DMSO-d₆.