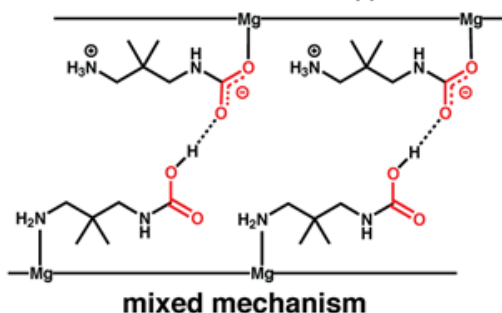
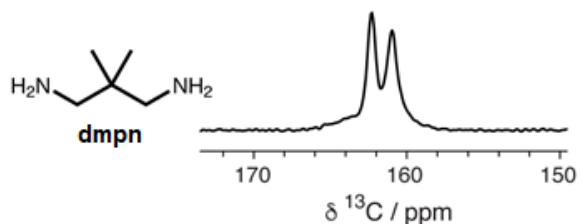
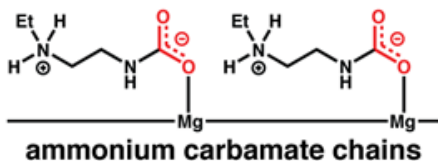
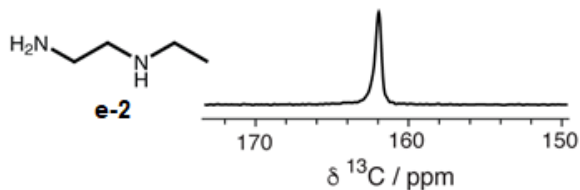


# Elucidating CO<sub>2</sub> Chemisorption in Diamine-Appended Metal–Organic Frameworks



<sup>13</sup>C solid-state NMR spectra of amine functionalized Mg<sub>2</sub>(dobpdc) MOFs dosed with CO<sub>2</sub> and chemisorption mechanisms. Top: e-2–Mg<sub>2</sub>(dobpdc), bottom: dmpn–Mg<sub>2</sub>(dobpdc)

## Scientific Achievement

Determination of CO<sub>2</sub> chemisorption mechanisms in 13 diamine-appended metal–organic frameworks (MOFs), and discovery of a new mixed ammonium carbamate – carbamic acid adsorption mechanism.

## Significance and Impact

Diamine-appended MOFs are promising materials for CO<sub>2</sub> capture, but elucidating adsorption mechanisms and designing new materials has remained challenging. Our new toolkit for assessing CO<sub>2</sub> chemisorption mechanisms can be applied broadly to CO<sub>2</sub> capture materials.

## Research Details

- Hardware made to study CO<sub>2</sub>-dosed samples by NMR.
- Combining solid state NMR spectra and DFT calculations enabled determination of CO<sub>2</sub> chemisorption mechanisms.

Forse, A. C.; Milner P. J.; Lee, J.-H.; Redfearn, H. N.; Oktawiec, J.; Siegelman, R. L.; Martell, J. D.; Dinakar, B; Porter-Zasada, L. B.; Gonzalez, M. I.; Neaton, J. B.; Long, J. R.; Reimer, J. A. *J. Am. Chem. Soc.* **2018**, *140*, 18016.

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