

Supplemental Materials for: Activating Magnesium Electrolytes through Chemical Formation of Free Chloride and Removal of Trace Water

Seong Shik Kim and Kimberly A. See*

*Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena,
California 91125, United States*

E-mail: ksee@caltech.edu

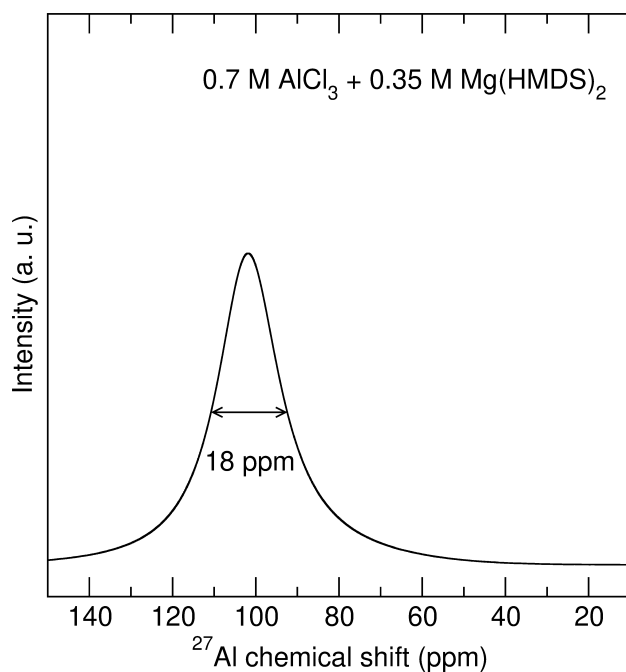


Figure S1: ^{27}Al NMR of $0.7\text{ M AlCl}_3 + 0.35\text{ M Mg(HMDS)}_2$. Only one broad resonance is observed at 102 ppm with a full width at half maximum of 18 ppm.

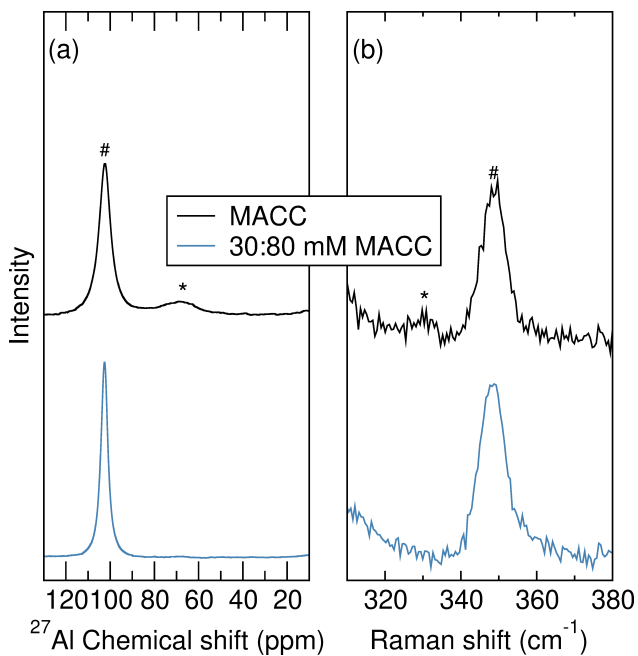


Figure S2: (a) ^{27}Al NMR and (b) Raman spectra of MACC and 30:80 mM MACC. The 66 ppm resonance present in MACC (*), which corresponds to AlCl_3 , is not present in 30:80 mM MACC. Similarly, the Al–Cl mode of AlCl_3 at 328 cm^{-1} present in MACC (*) is not present in 30:80 mM MACC.

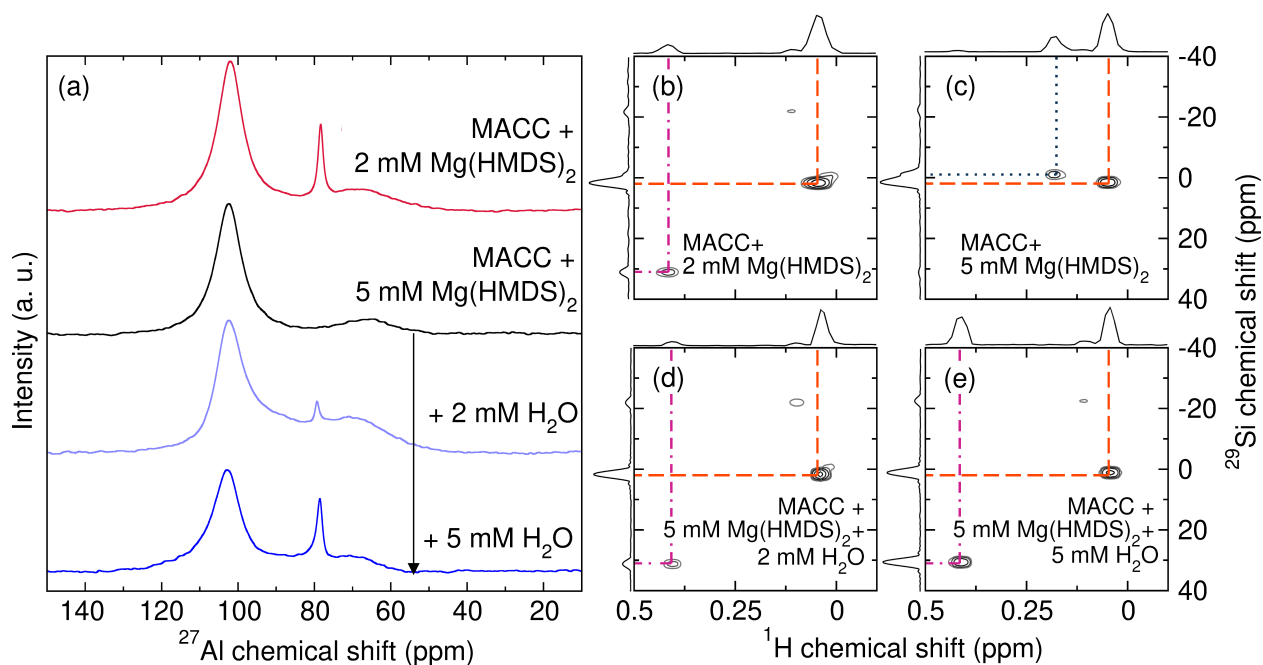


Figure S3: (a) ^{27}Al NMR spectra and ^1H - ^{29}Si HMBC spectra of MACC (b) + 2 mM $\text{Mg}(\text{HMDS})_2$, (c) + 5 mM $\text{Mg}(\text{HMDS})_2$, (d) + 5 mM $\text{Mg}(\text{HMDS})_2$ + 2 mM H_2O , (e) + 5 mM $\text{Mg}(\text{HMDS})_2$ + 5 mM H_2O . The 78 ppm resonance in ^{27}Al NMR and the {0.415, 31} ppm cross peak in ^1H - ^{29}Si HMBC are not present in MACC + 5 mM $\text{Mg}(\text{HMDS})_2$, but appear in the presence of H_2O .

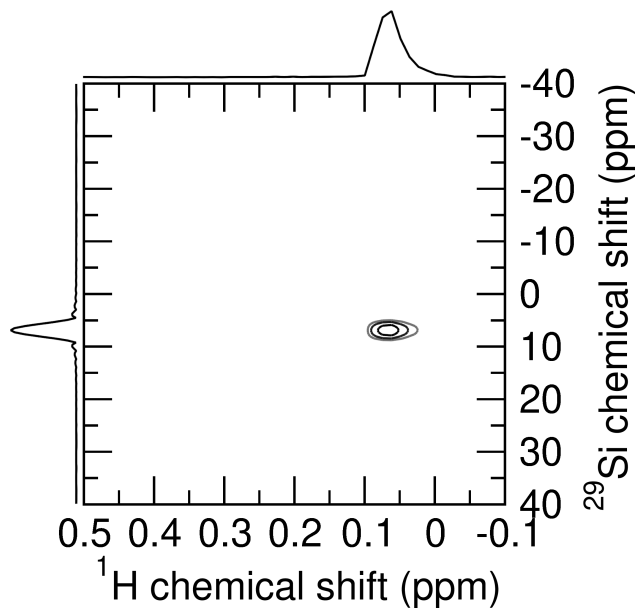


Figure S4: ^1H - ^{29}Si HMBC spectrum of trimethylsilanol ($(\text{CH}_3)_3\text{SiOH}$), whose cross peak is located at {0.066, 7} ppm.

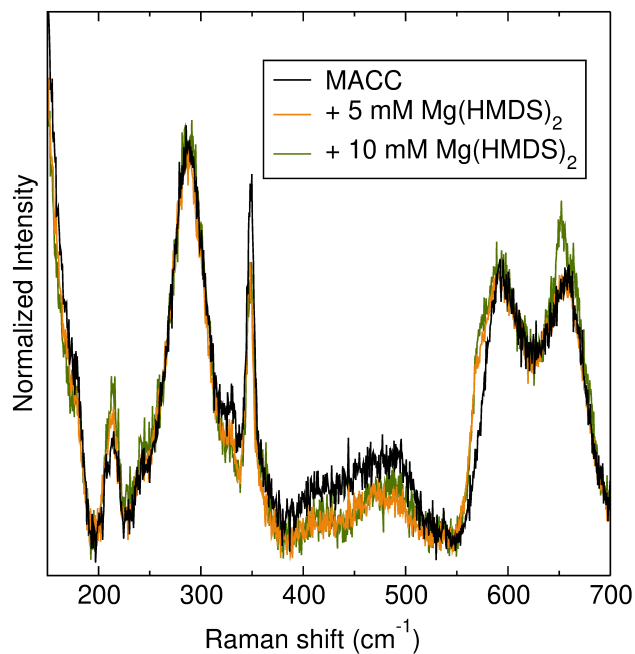


Figure S5: Raman spectra of as-prepared MACC, MACC + 5, and 10 mM Mg(HMDS)₂ overlaid on top of one another. These spectra are the same spectra as in Figure 1. All intensities are normalized to a THF mode at 913 cm⁻¹. With increasing Mg(HMDS)₂ concentration, the [Mg₂(μ-Cl)₃·6(THF)]⁺ mode at 210 cm⁻¹ increases while the AlCl₄⁻ mode at 347 cm⁻¹ decreases in intensity. Also, two new modes develop at 569 cm⁻¹ and 651 cm⁻¹.