

Article

# Supplementary Material for "Tracking Amorphous Calcium Carbonate Crystallization Products with Far-Infrared Spectroscopy"

Boyang Gao<sup>1</sup> and Kristin M. Poduska<sup>1,2\*</sup>

<sup>1</sup> Department of Chemistry, Memorial University of Newfoundland & Labrador, St. John's, NL, A1C 5S7, Canada

<sup>2</sup> Department of Physics & Physical Oceanography, Memorial University of Newfoundland & Labrador, St. John's, NL, A1B 3X7, Canada

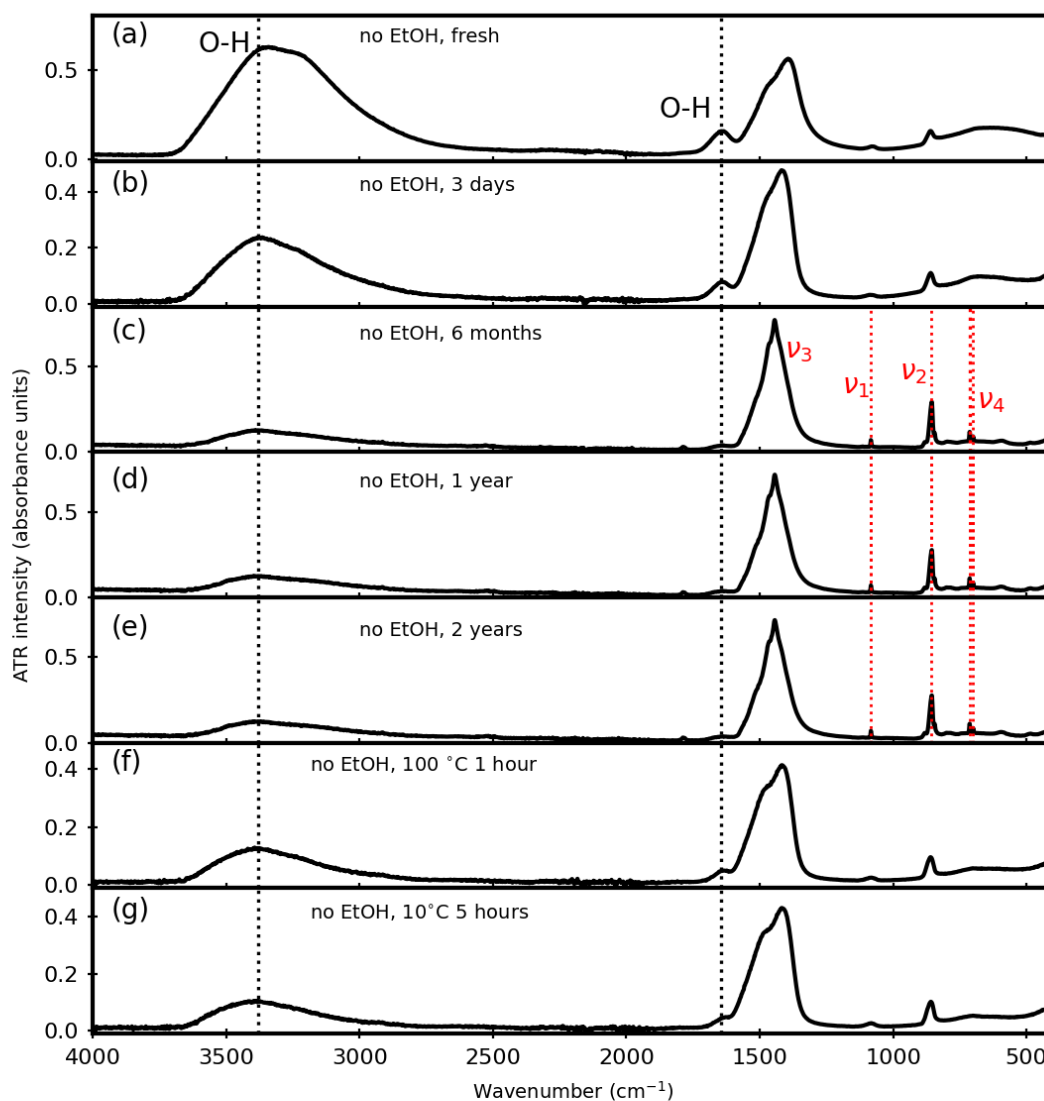
\* Correspondence: kris@mun.ca

Version January 10, 2023 submitted to Minerals

---

To illustrate the time-dependent changes that occur in samples prepared without ethanol (no EtOH), we compare representative mid-infrared (MIR) attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectra of fresh solids (Figure S1a) with ambient-aged solids (Figure S1b,c,d,e). The water-related peaks (OH-stretching near  $3400\text{ cm}^{-1}$  and OH-bending near  $1600\text{ cm}^{-1}$ ) decrease after days to years under ambient conditions. These same water-related peaks decrease noticeably after heating (Figure S1f,g), but do not disappear completely. Furthermore, heating does not trigger aragonite formation.

© 2023 by the authors. Submitted to *Minerals* for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).



**Figure S1.** Representative ATR-FTIR spectra in the mid-IR range ( $400\text{--}4000\text{ cm}^{-1}$ ) for samples synthesized without EtOH (a) fresh, and after different periods of drying in ambient: (b) 3 days, (c) 6 months, (d) 1 year, (e) 2 years. For comparison, fresh samples were also heated to  $100\text{ }^{\circ}\text{C}$  for (f) 1 h, and (g) 5 h. The black dotted lines indicate water-related peaks (OH-stretching near  $3400\text{ cm}^{-1}$  and OH-bending near  $1600\text{ cm}^{-1}$ ) while the red dotted lines correspond to the most diagnostic aragonite-specific peaks ( $\nu_1$  peak region (near  $1080\text{ cm}^{-1}$ ),  $\nu_2$  peak region ( $800\text{--}920\text{ cm}^{-1}$ ) and  $\nu_4$  peak region ( $650\text{--}800\text{ cm}^{-1}$ )).