

Supporting information (SI) for:

Ice Nucleation at the Water-Sapphire Interface: Transient Sum Frequency Response without Evidence for Transient Ice Phase

Ahmed Abdelmonem,^{a} Ellen H. G. Backus^b and Mischa Bonn^{b*}*

^aInstitute of Meteorology and Climate Research – Atmospheric Aerosol Research (IMKAAF), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

^bMax Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

*E-mail: ahmed.abdelmonem@kit.edu, bonn@mpip-mainz.mpg.de

Non-Fresnel Corrected Spectra of Figure 1:

Figure S1 shows the non-Fresnel corrected SFG spectra of Figure 1.

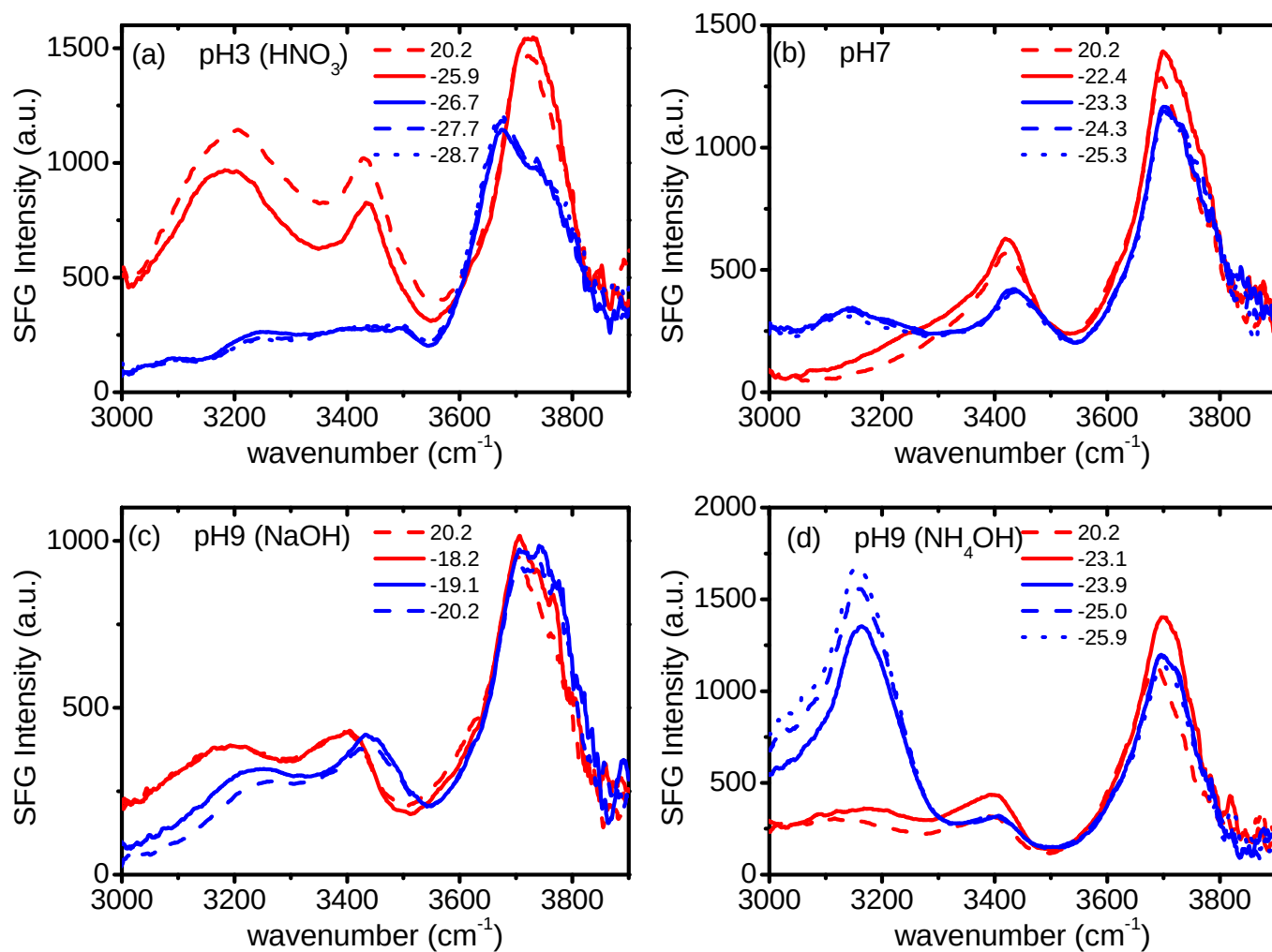
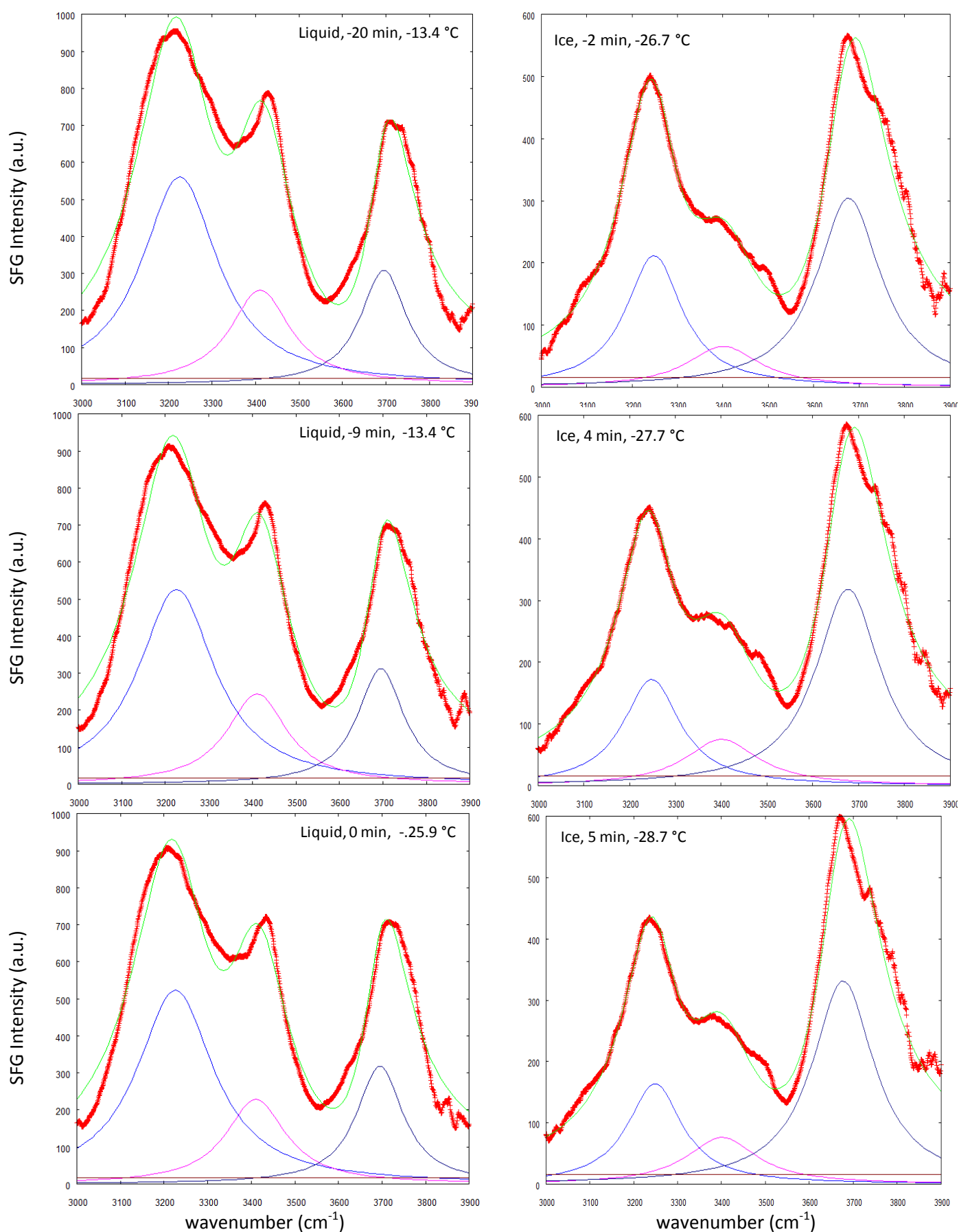


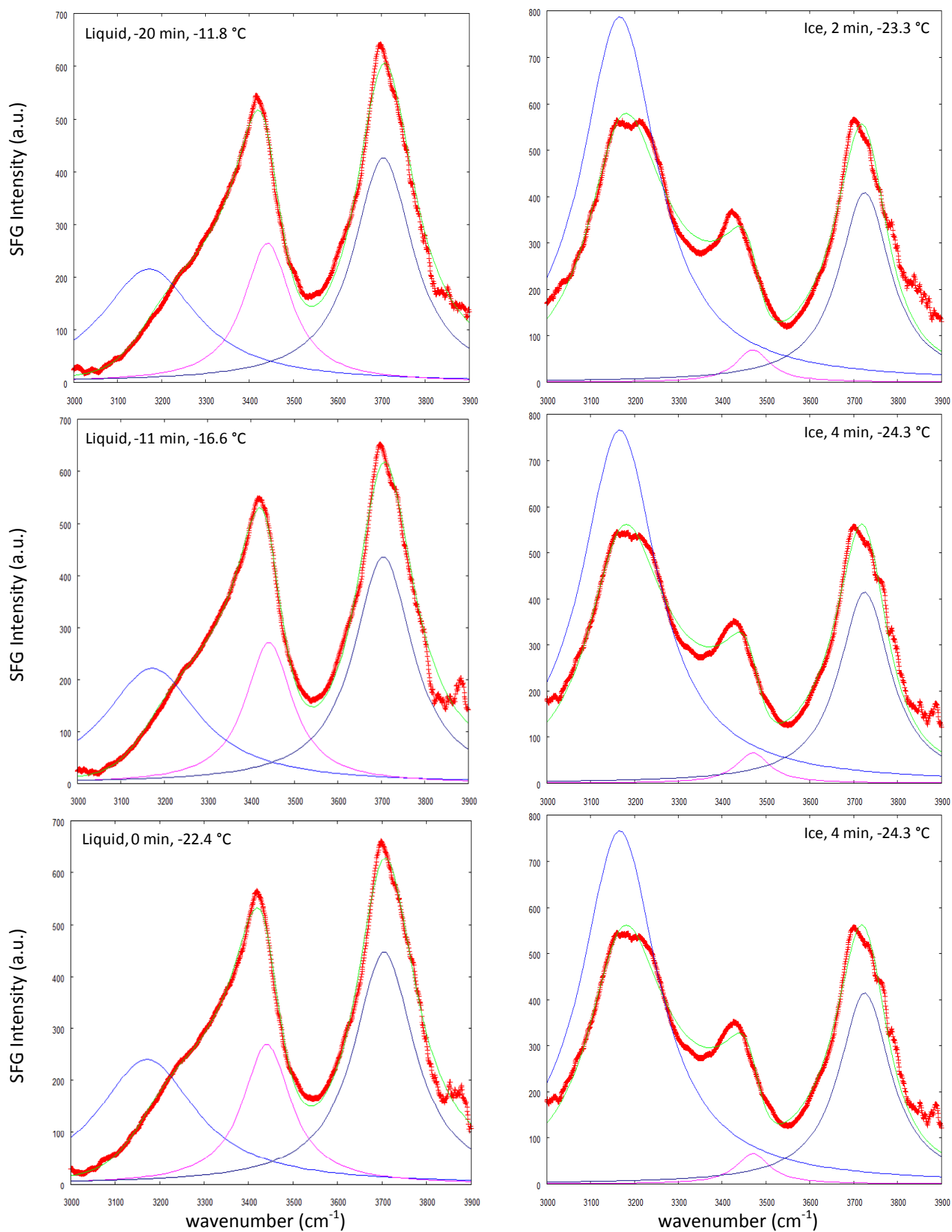
Figure S1 Non-Fresnel corrected SFG spectra of Figure 1. (a) pH 3 - HNO₃, (b) pH 7, (c) pH 9 - NaOH and (d) pH 9 - NH₄OH.

Spectra fit Samples:

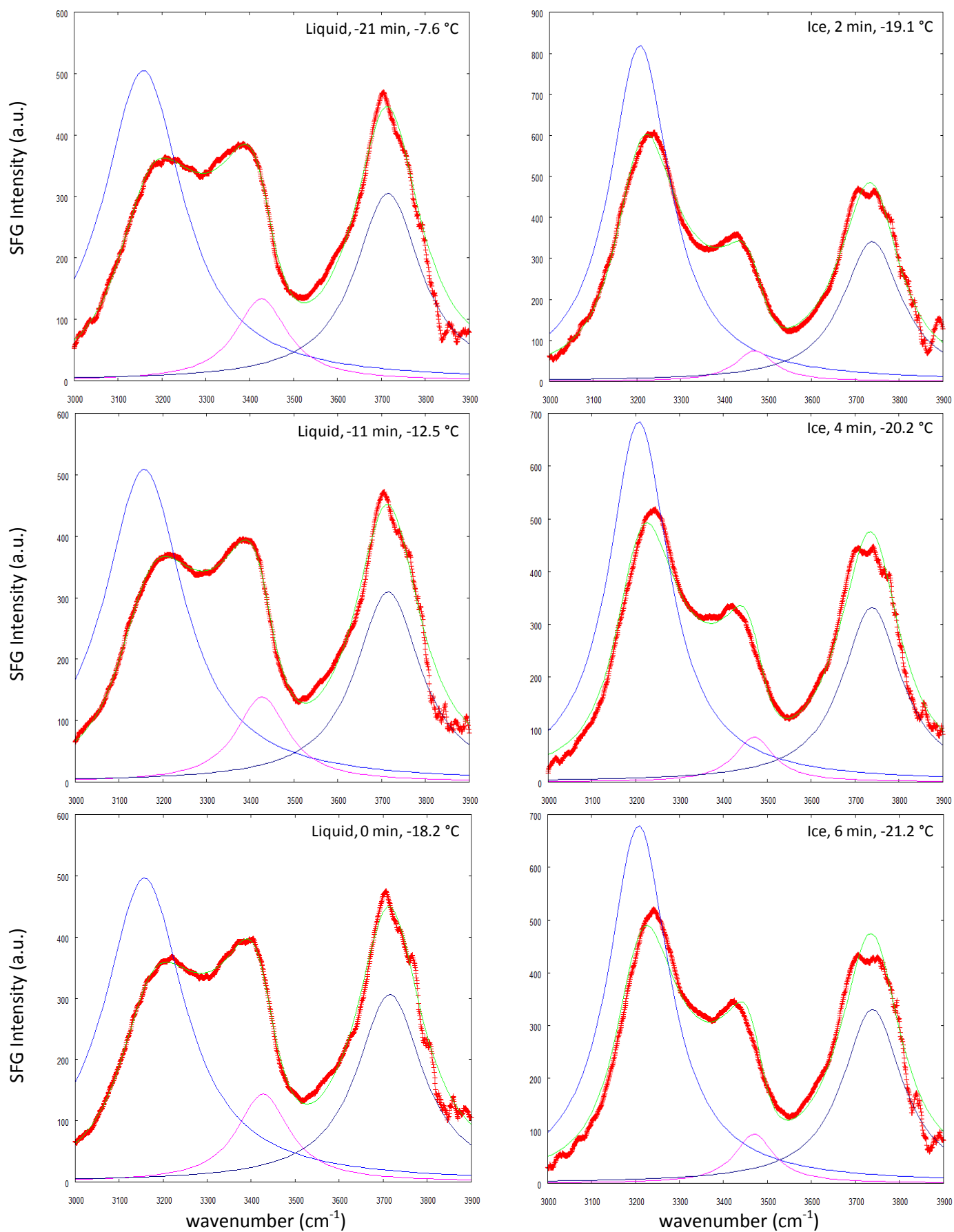
Figure S2 shows some examples of the fitting results around the freezing point (time zero) to demonstrate the fit quality.



(a) pH 3 (HNO₃),



(b) pH 7



(c) pH 9 (NaOH)

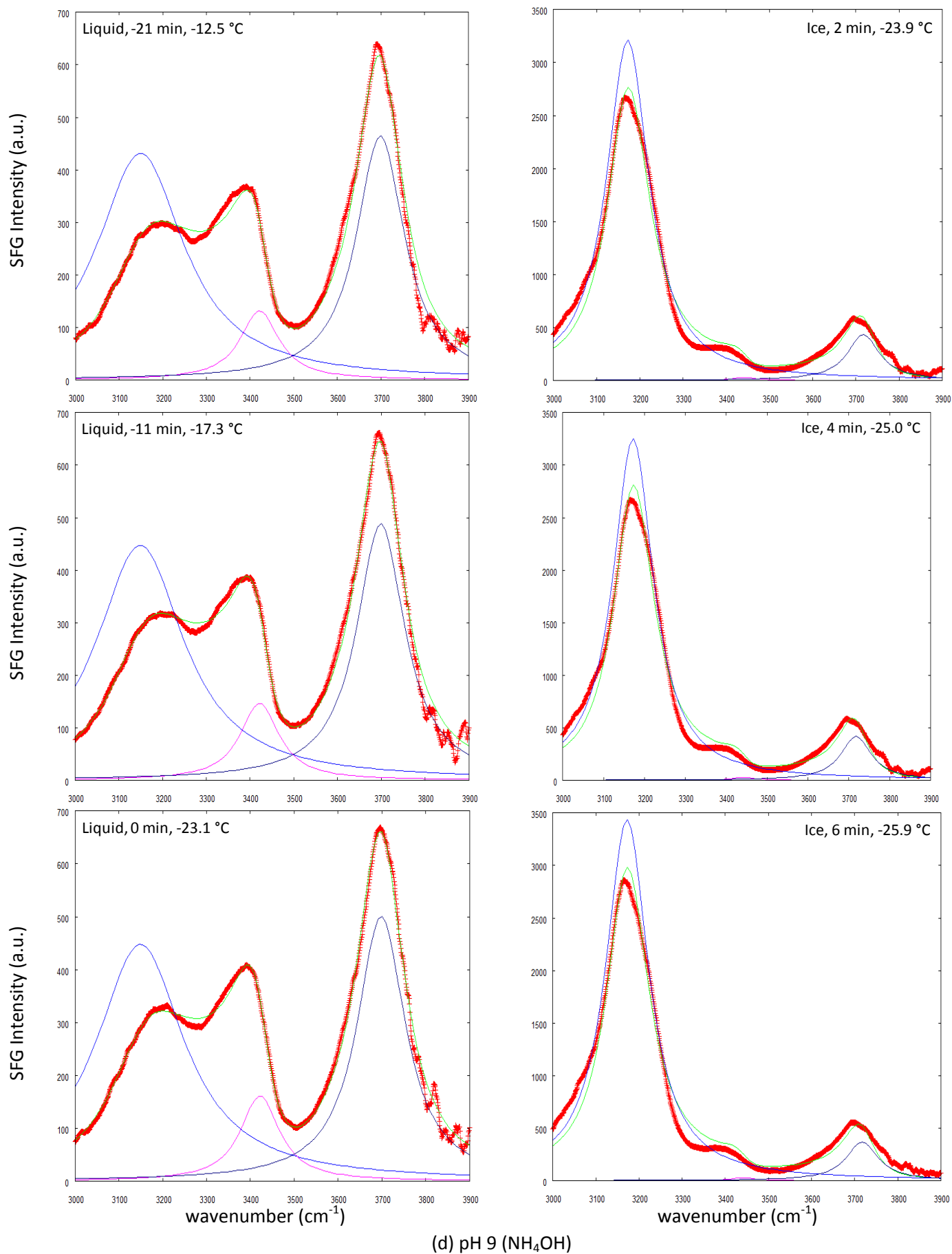
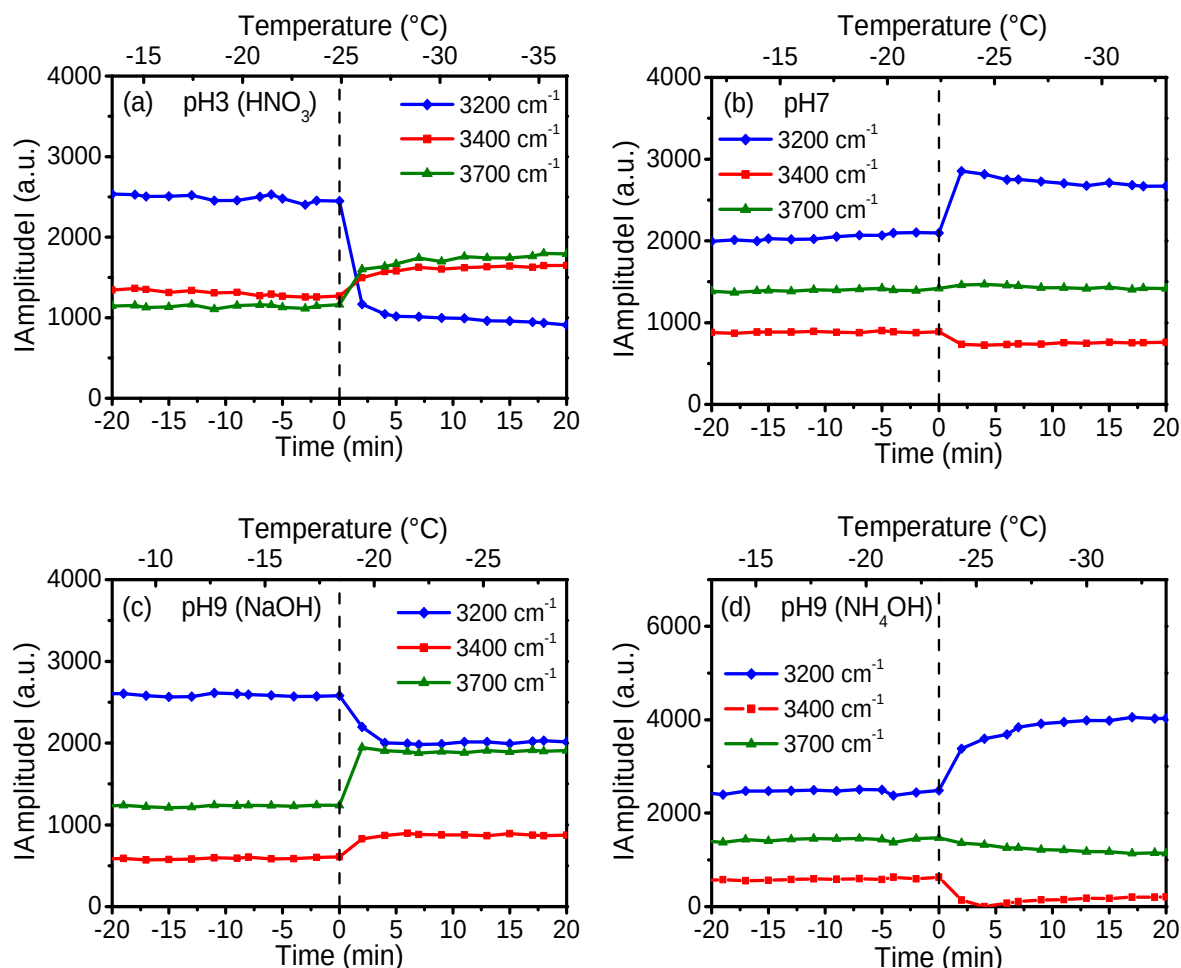


Figure S2 a. Samples of the fitting results. (a) pH 3 (HNO_3), (b) pH 7, (c) pH 9 (NaOH) and (d) pH 9 (NH_4OH). The label on each panel shows the water phase, the time with respect to the freezing point and the temperature.

Fitting parameters:

The center frequencies and linewidths of the resonances and the amplitude and phase of the nonresonant background were kept constant for each phase (liquid and ice) in the fit procedure used to plot Figure 3. In Figure S3 we show two examples of different fitting procedures. Figure S3a shows an example where the center frequencies and linewidths of the resonances were kept constant, while the amplitude and phase of the nonresonant background were allowed to change upon phase change (liquid/ice) but fixed during the fitting iterations within the same phase. Figure S3b shows an example of non-constrained fitting for pH9 (NaOH) where all parameters were allowed to change during the fitting iterations. The different fit routines result in subtle changes not affecting any conclusions.

(a)



(b)

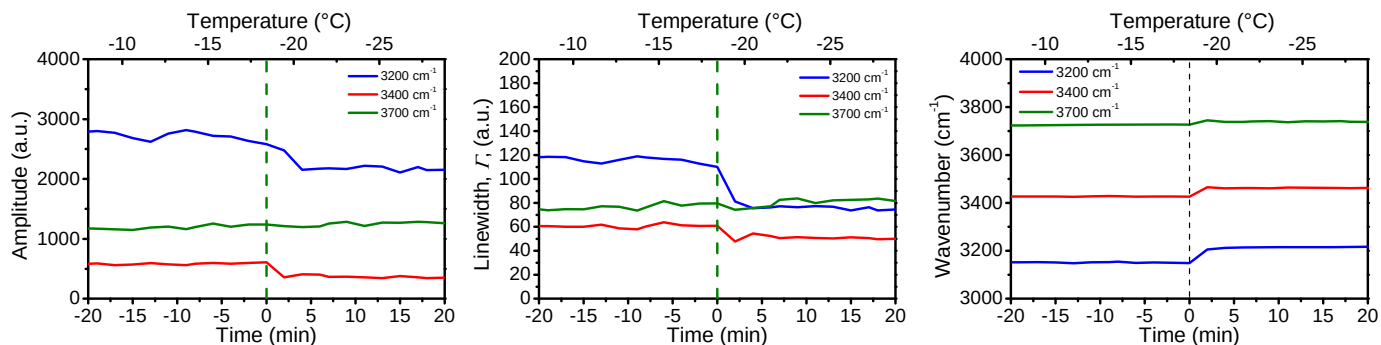


Figure S3 Two examples of different fitting procedures. (a) Absolute peak amplitude of individual bands for all solutions under fixed frequency and linewidth of the resonances, and free amplitude and phase of the nonresonant background during the fitting iterations. (b) A plot of the individual fit parameters as a function of time/temperature for pH9 (NaOH) which are obtained from the non-constrained fit procedure.