

Exploring the Thermal Reversibility and Tunability of a Low Molecular Weight Gelator using Vibrational and Electronic Spectroscopy and Rheology

Supporting Information

*David DiGuisseppi¹, Lavenia Thursch², Nicolas Alvarez², and
Reinhard Schweitzer-Stenner^{1*}*

¹Department of Chemistry and ²Department of Chemical and Biological
Engineering, Drexel University, Philadelphia, PA 19104, USA

To be submitted to: Soft Matter

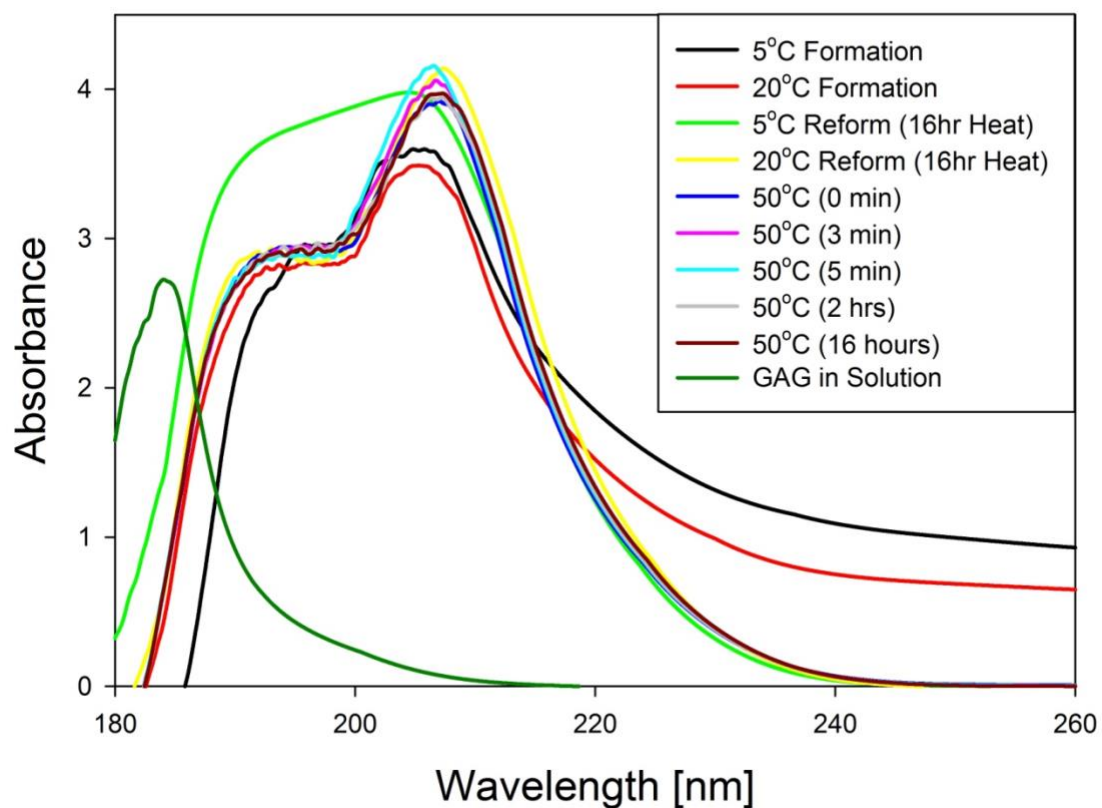


Figure S1. Absorbance spectra of the cationic GAG in 55mol %ethanol/45mol% water in the sol phase (Solution), gel phase I (5° C), gel phase II (20° C), at elevated temperature and after an annealing process involving a residence time of 16 h at 50°C. The final temperatures of the respective annealing cycles are indicated.

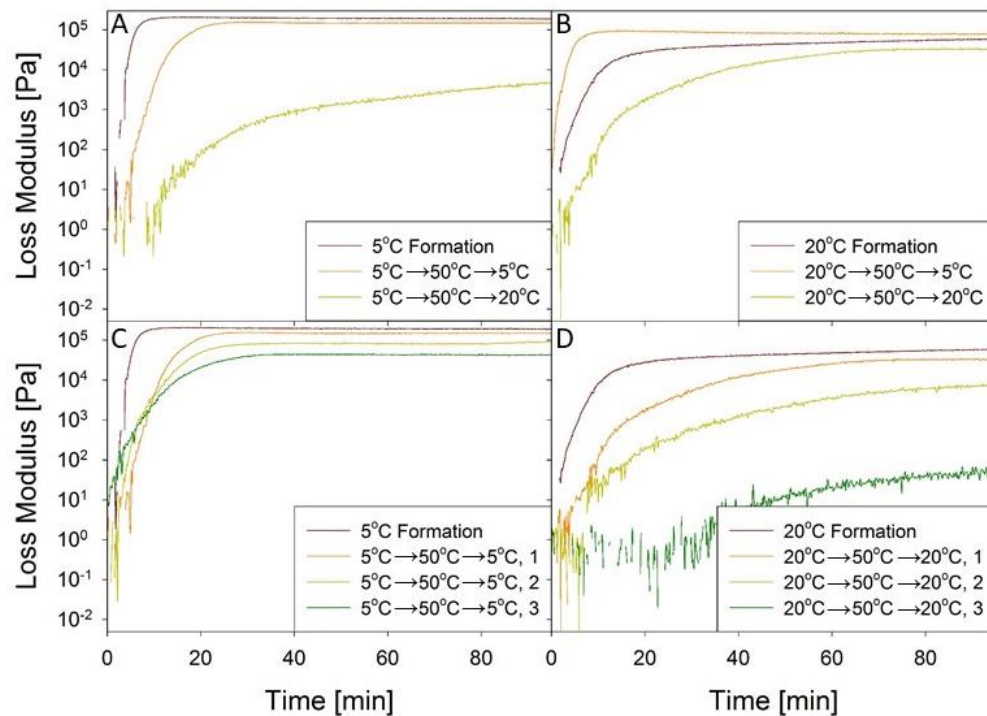


Figure S2. Kinetics of gel formation of cationic GAG in 55 mol% ethanol/45 mol% water at indicated temperatures and gel reformation after the indicated annealing processes measured by the loss modulus G'' . The respective kinetics probed by the storage modulus are shown in Figure 2 of the main manuscript.

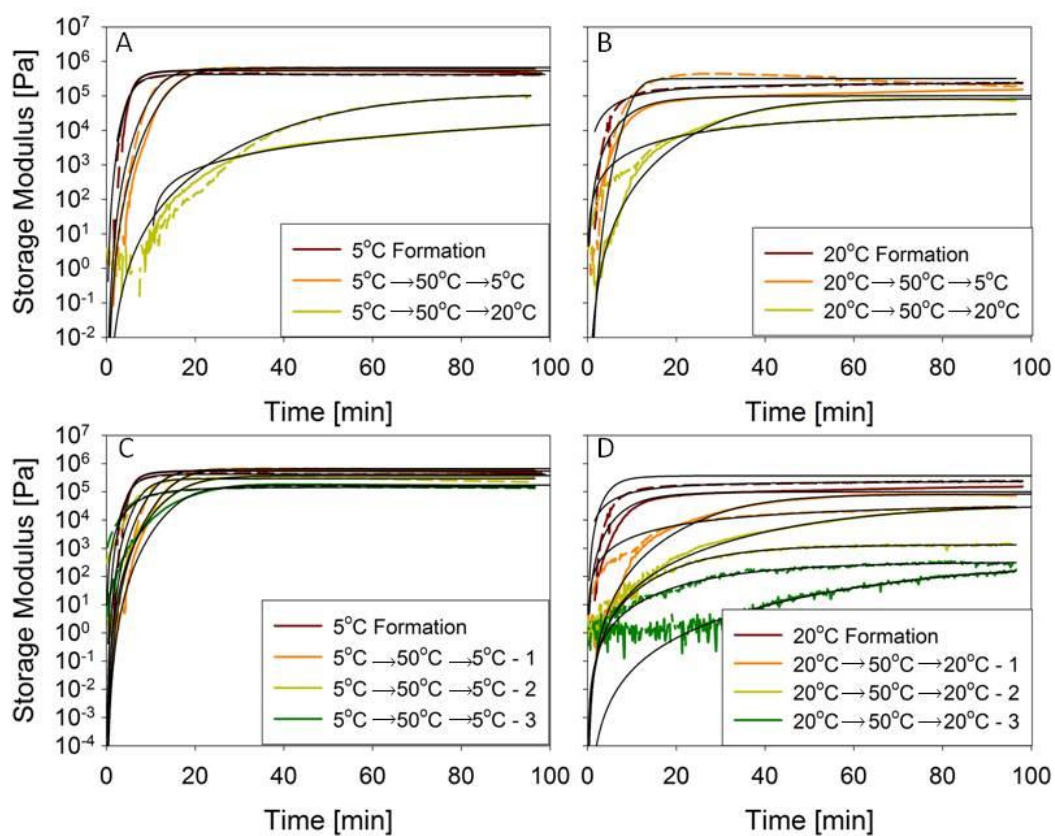


Figure S3. Replicate measurements of the formation and reformation G' kinetics correlating to Figure 3. The solid colored lines are from one trial and the dashed are another. The solid black lines are the obtained fits that are discussed in the text.

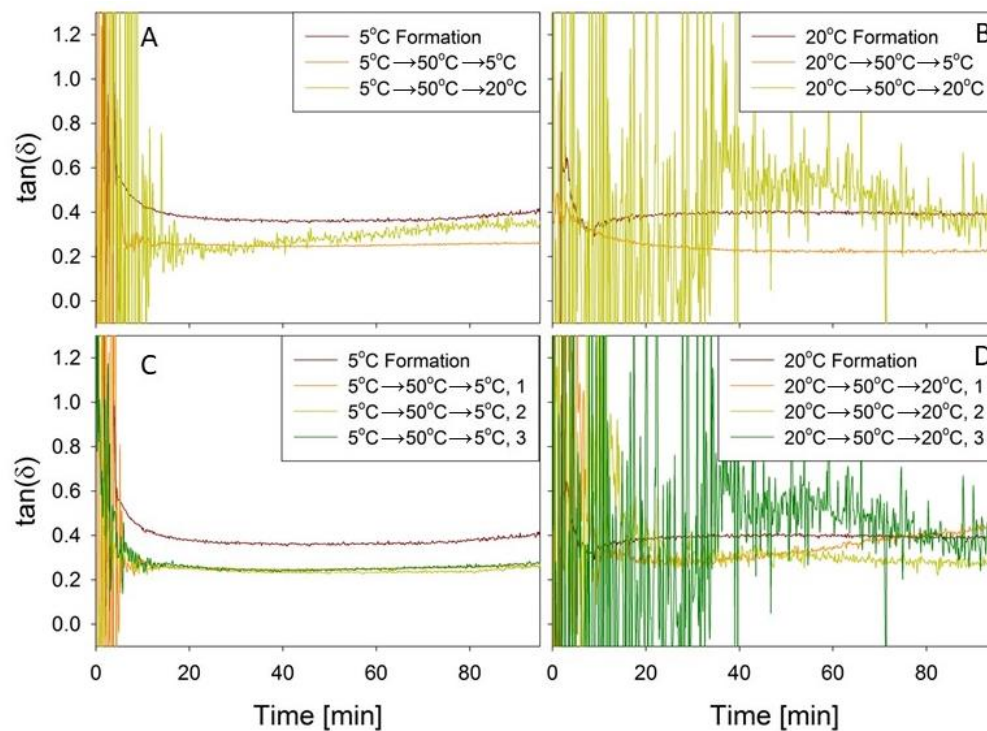


Figure S4. Time dependence of $\tan \delta$ during the gel formation of cationic GAG in 55 mol% ethanol/45 mol% water at indicated temperatures and the gel reformation after the indicated annealing processes measured by the loss modulus G'' . The respective kinetics probed by the storage modulus G' are shown in Figure 2 of the main manuscript.

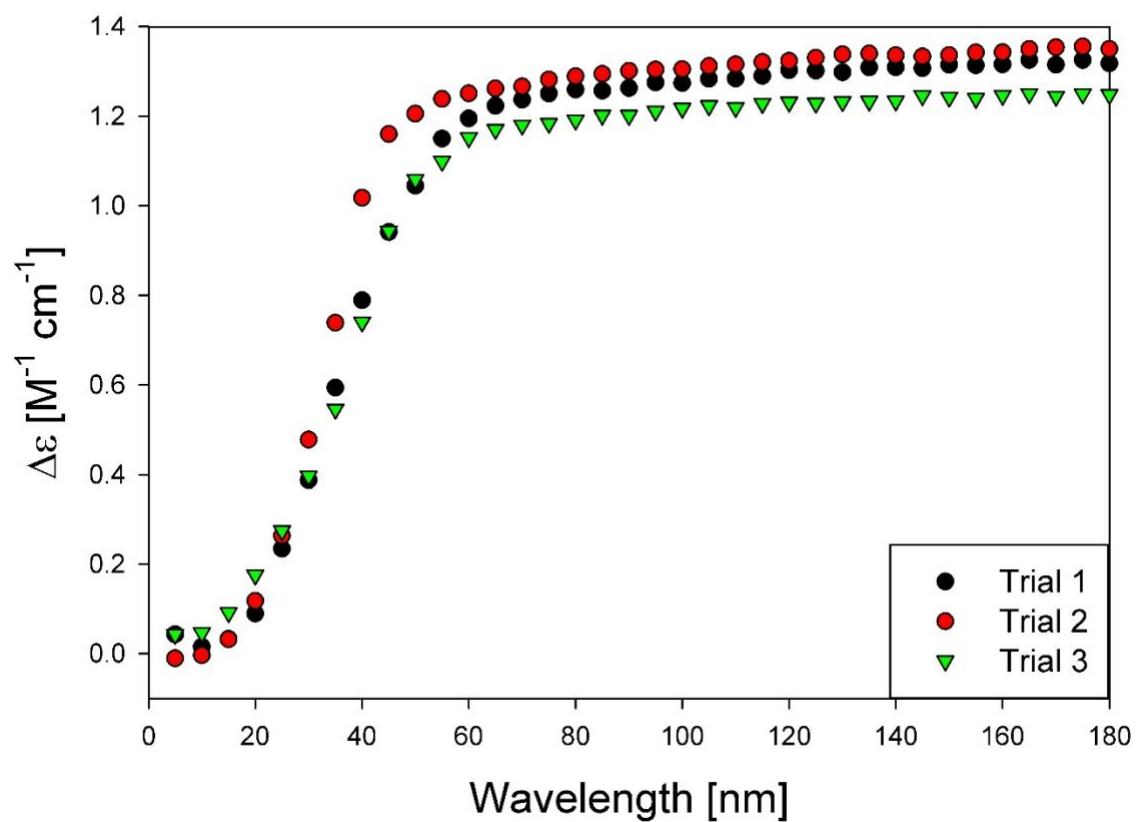


Figure S5. $\Delta\epsilon_{221}$ values obtained from ECD for replicate measurements of samples formed at 5°C, heated to 50°C for five minutes, and reformed at 5°C.

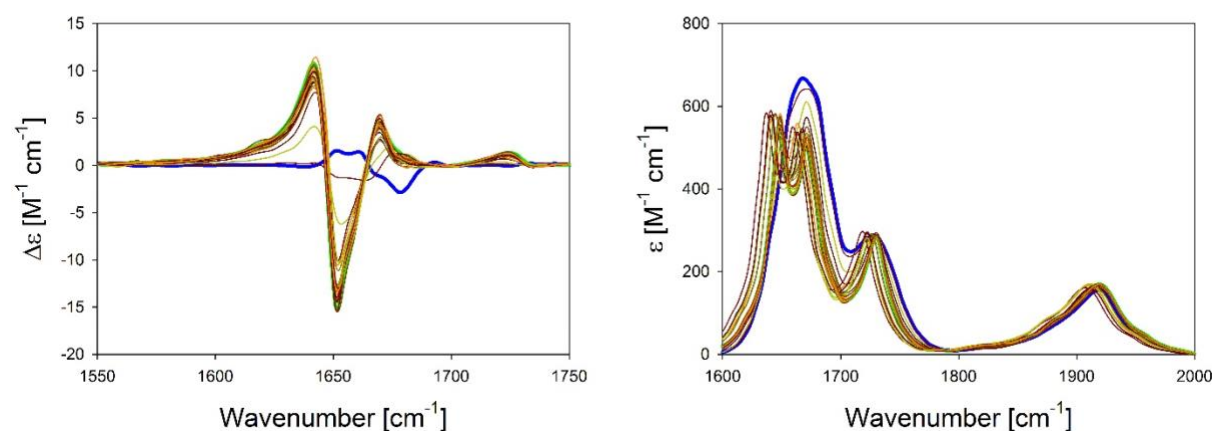


Figure S6. Amide I' region of the VCD and IR spectra of cationic GAG in 55 mol% ethanol/45 mol% water recorded every five minutes over a period of two hours while the sample formed a gel at 5°C and reformed at 5°C after annealing. The bolded-blue spectra were taken after 5 minutes. The bolded-green spectra were recorded after 120 minutes.

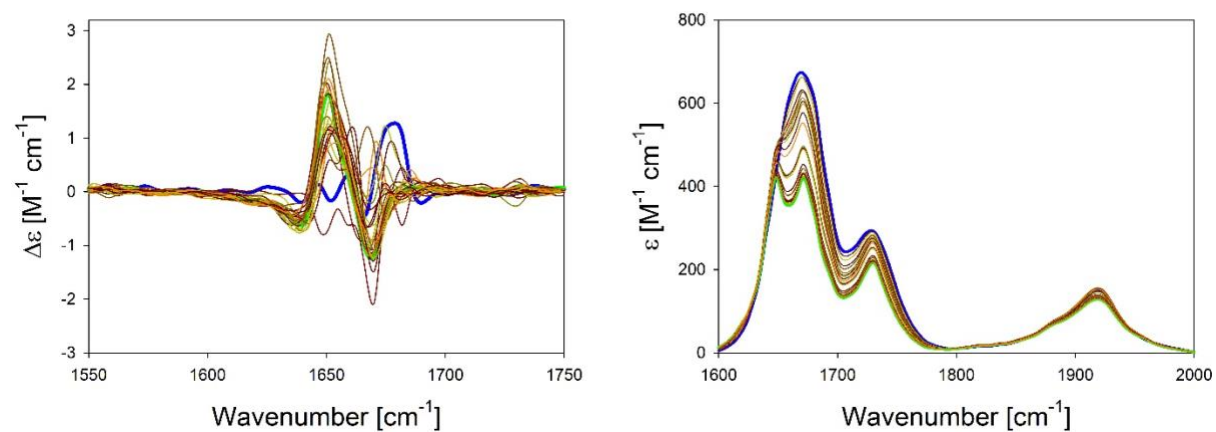


Figure S7. Amide I' region of the VCD and IR spectra of cationic GAG in 55 mol% ethanol/45 mol% water recorded every five minutes over a period of two hours while the sample formed a gel at 5°C and reformed at 20°C after annealing. The bolded-blue spectra were taken after 5 minutes. The bolded-green spectra were recorded after 120 minutes.

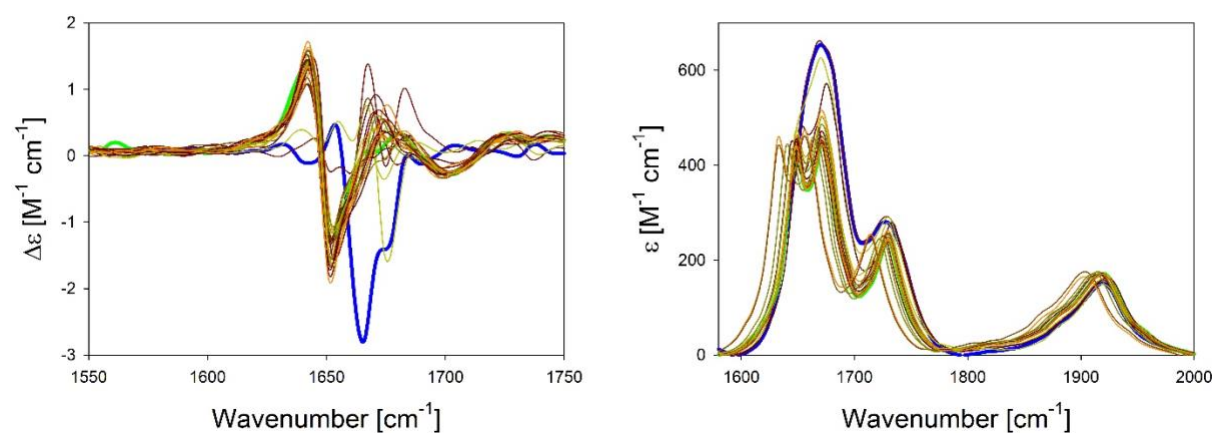


Figure S8. Amide I' region of the VCD and IR spectra of cationic GAG in 55 mol% ethanol/45 mol% water recorded every five minutes over a period of two hours while the sample formed the gel at 20°C and reformed at 5°C after annealing. The bolded-blue spectra were taken after 5 minutes. The bolded-green spectra were recorded after 120 minutes.

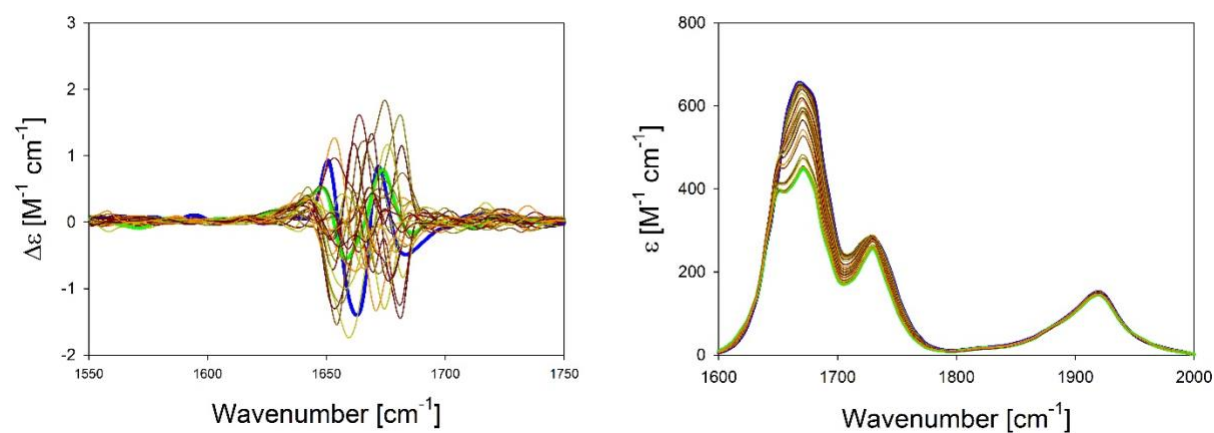


Figure S9. Amide I' region of the VCD and IR spectra of cationic GAG in 55 mol% ethanol/45 mol% water recorded every five minutes over a period of two hours while the sample formed the gel at 20°C and reformed at 20°C after annealing. The bolded-blue spectra were taken after 5 minutes. The bolded-green spectra were recorded after 120 minutes.

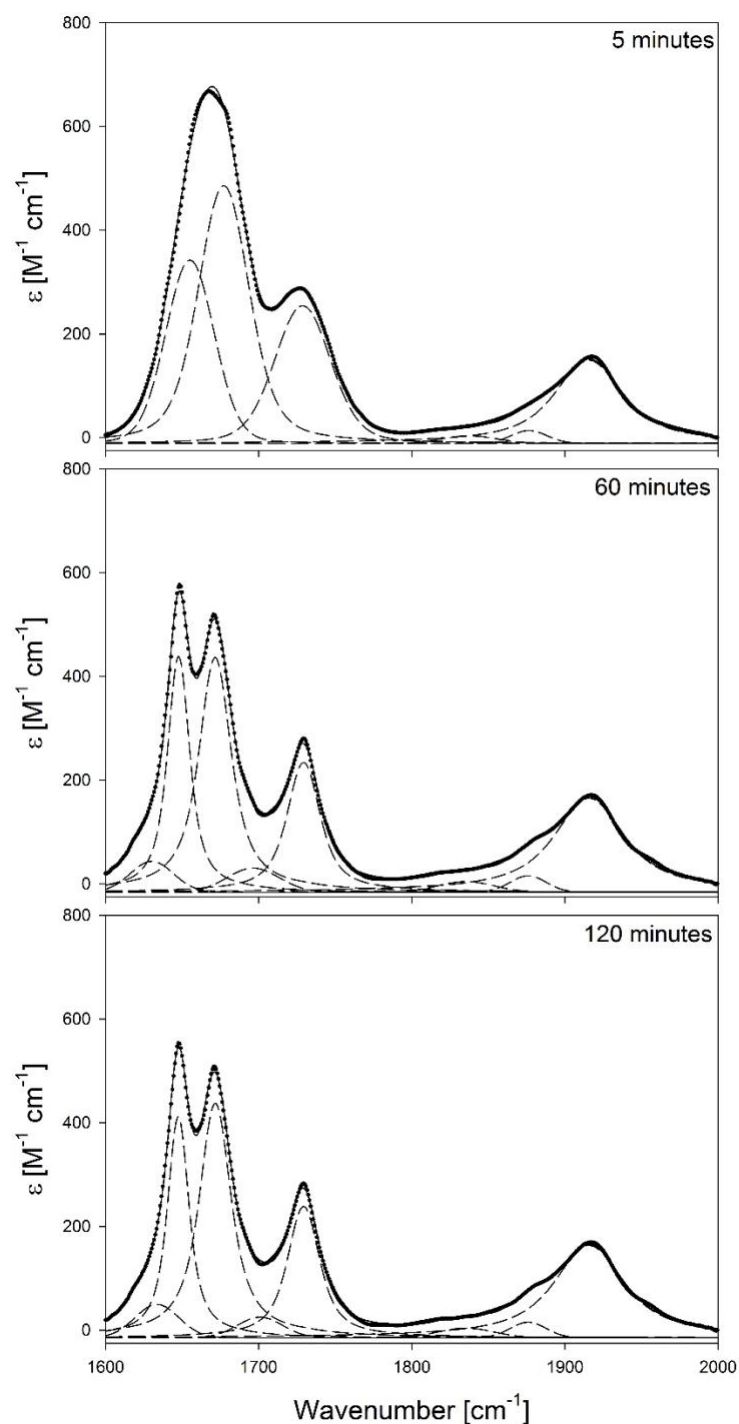


Figure S10. Spectral decomposition of IR spectra of the phase I gel of cationic GAG in 55 mol% ethanol/45 mol% water formed and subsequently reformed after annealing at 5°C recorded at three indicated times. The solid line represents the overall fit and the bolded points are experimental data points. Individual Gaussian and Lorentzian bands are depicted by dashed lines.

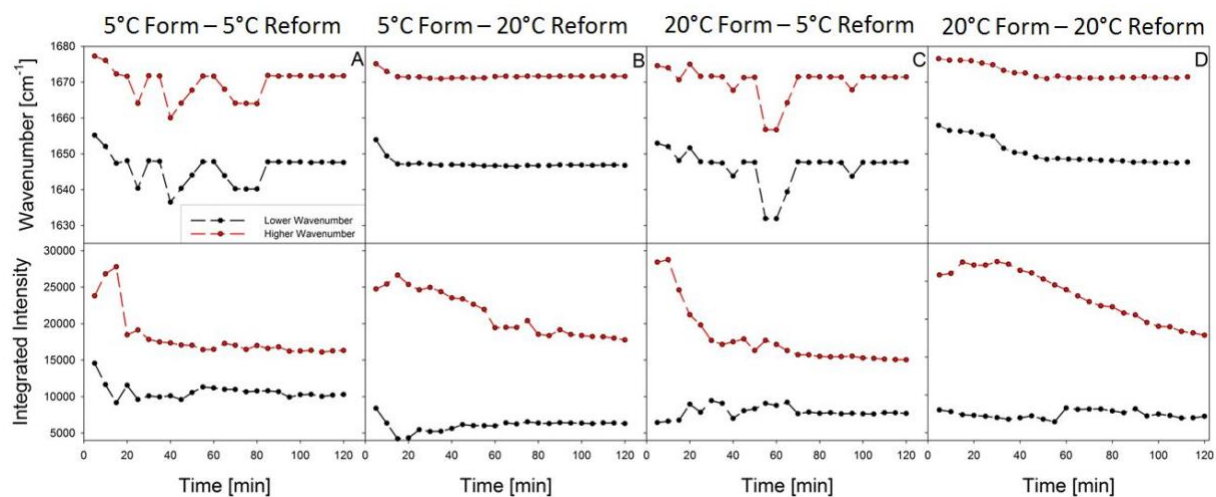


Figure S11. Time dependence of the wavenumber positions and integrated intensities of the two amide I' bands of cationic GAG in 55 mol% ethanol/45 mol% water obtained from the analysis of spectra taken after completion of the indicated annealing processes. The residence time at the elevated temperature was 5 minutes.

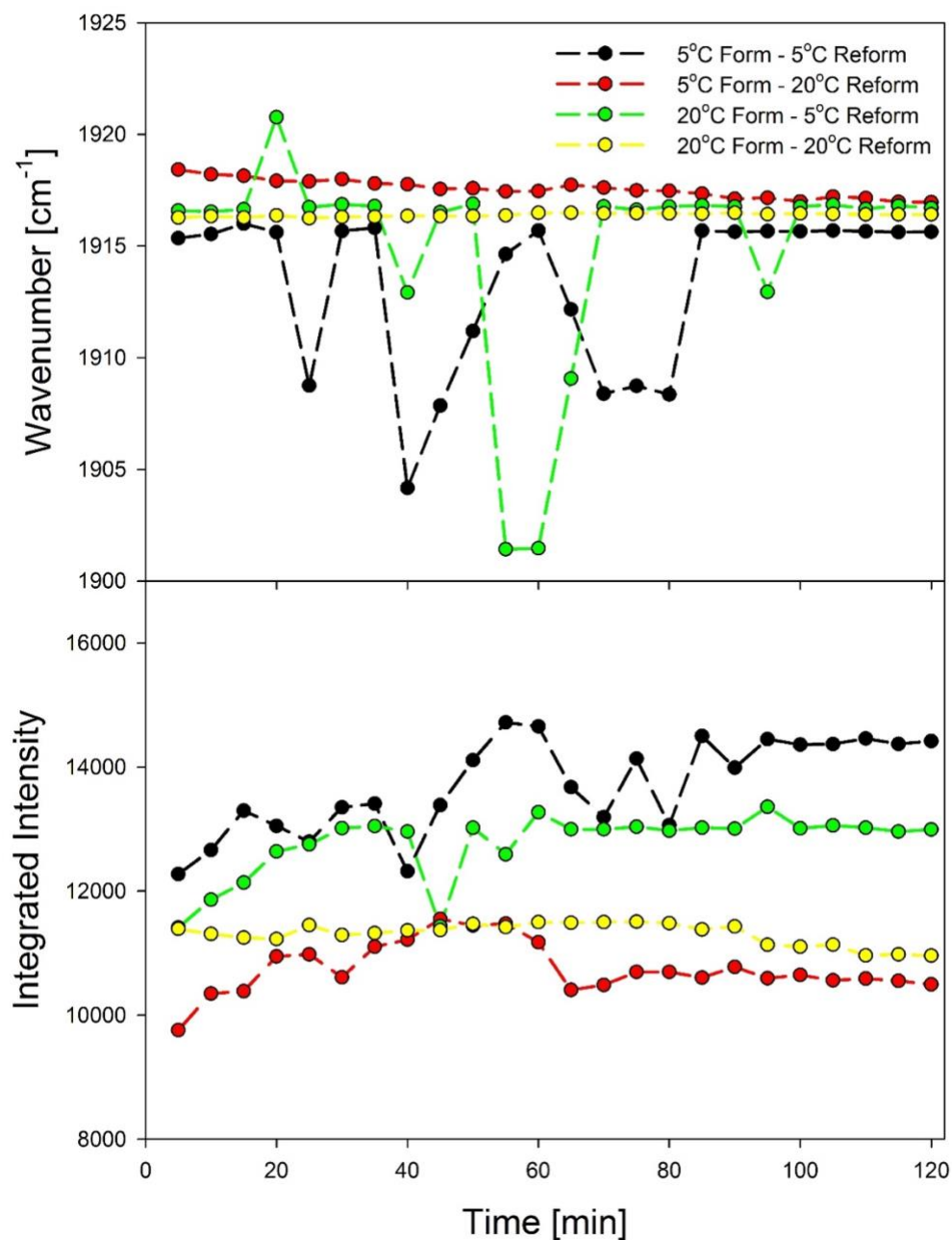


Figure S12. Time dependence of the wavenumber position and integrated intensity of the combination tone at 1910 cm⁻¹ of ethanol in ternary mixtures of 220 mM GAG/55 mol% ethanol/45 mol% water) obtained from the analysis of IR spectra taken after completion of the indicated annealing processes. The residence time at the elevated temperature was 5 minutes.

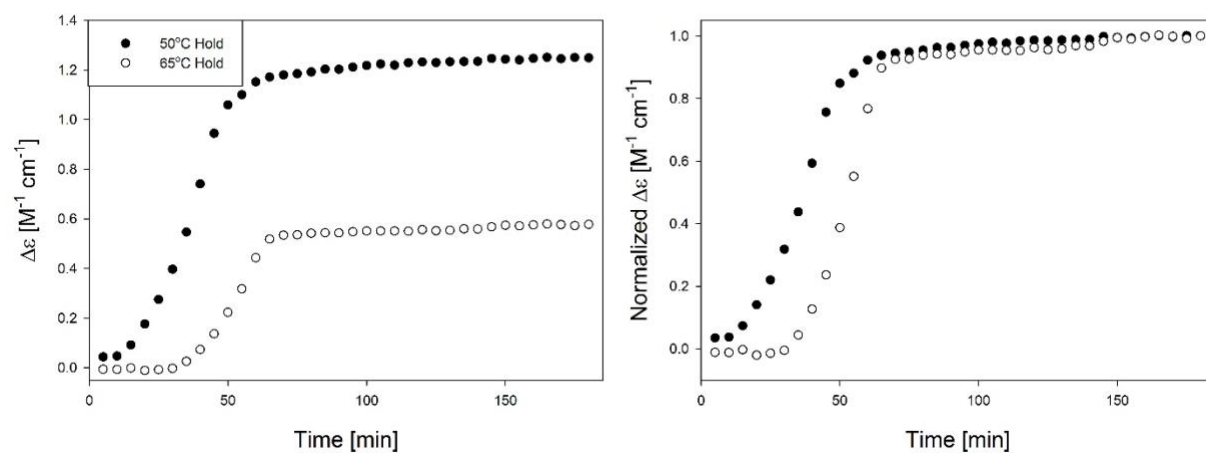


Figure S13. $\Delta\epsilon_{221}$ values obtained from ECD for samples formed at 5C, brought to 50C (filled) and 65C (empty) for five minutes, and then brought back down to 5C.

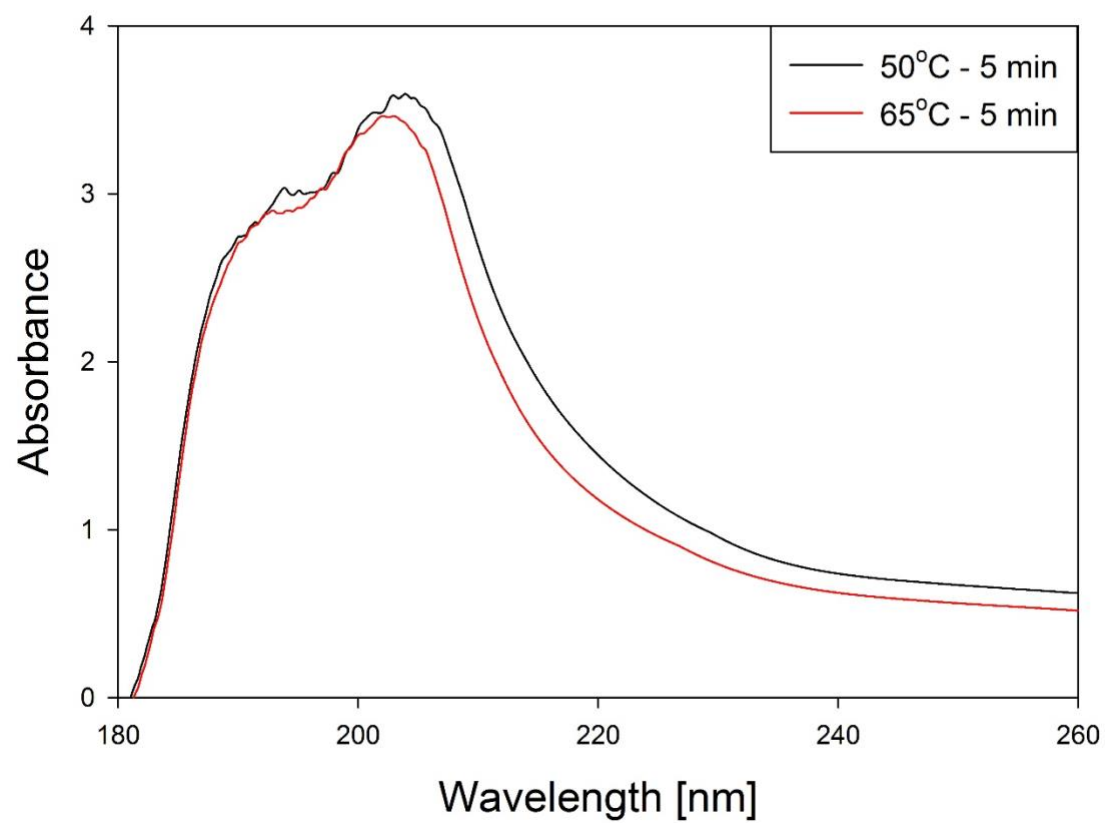


Figure S14. Absorbance spectra that correlate to the last data point from Figure S13.