Supplementary figures

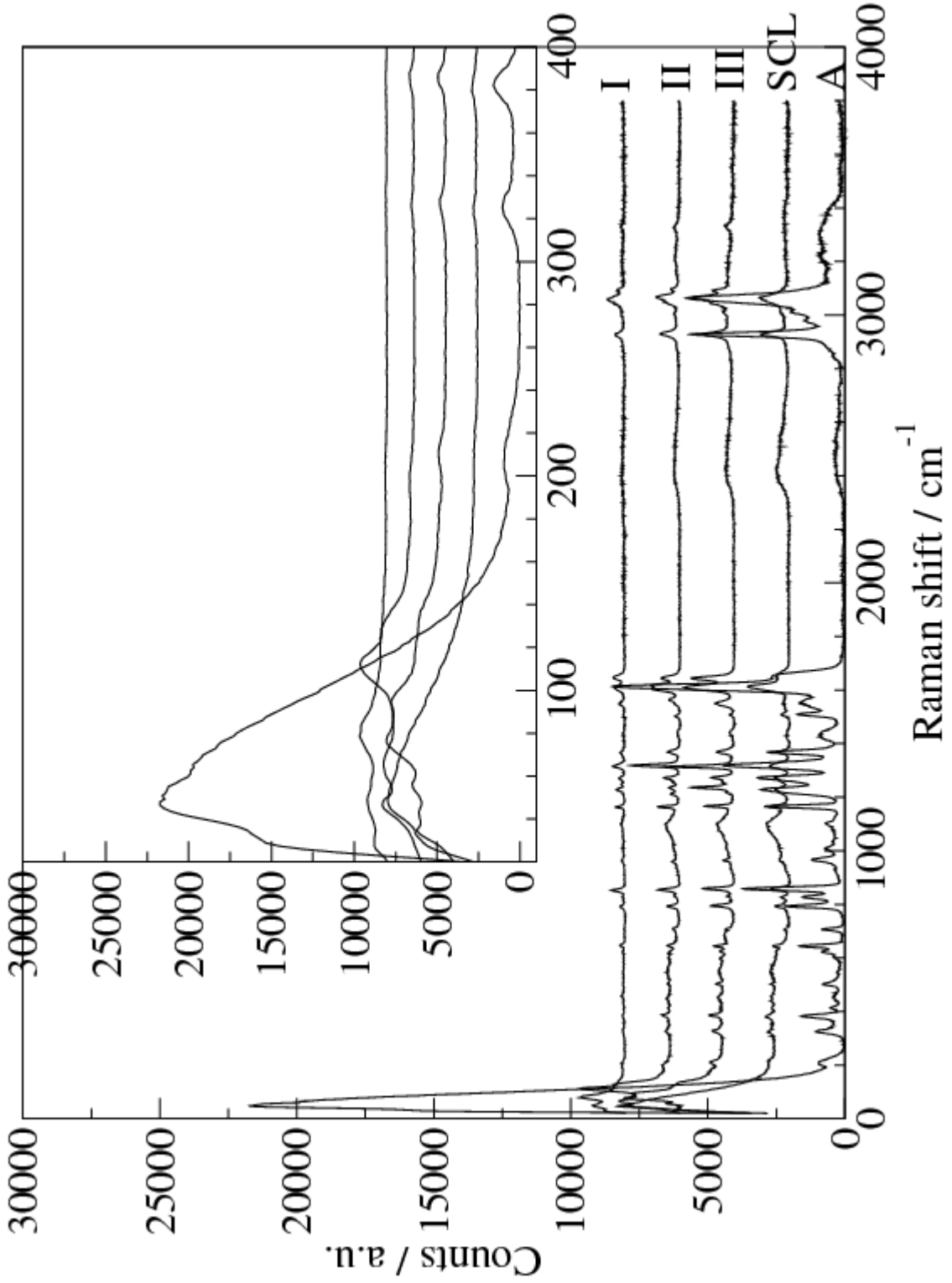

Figure S1: Example spectra (unscaled) for the different forms of paracetamol observed. A = amorphous, SCL = super-cooled liquid, III = Form III, etc.

Figure S2: Stacked plot of spectra (unscaled) across phase transitions.

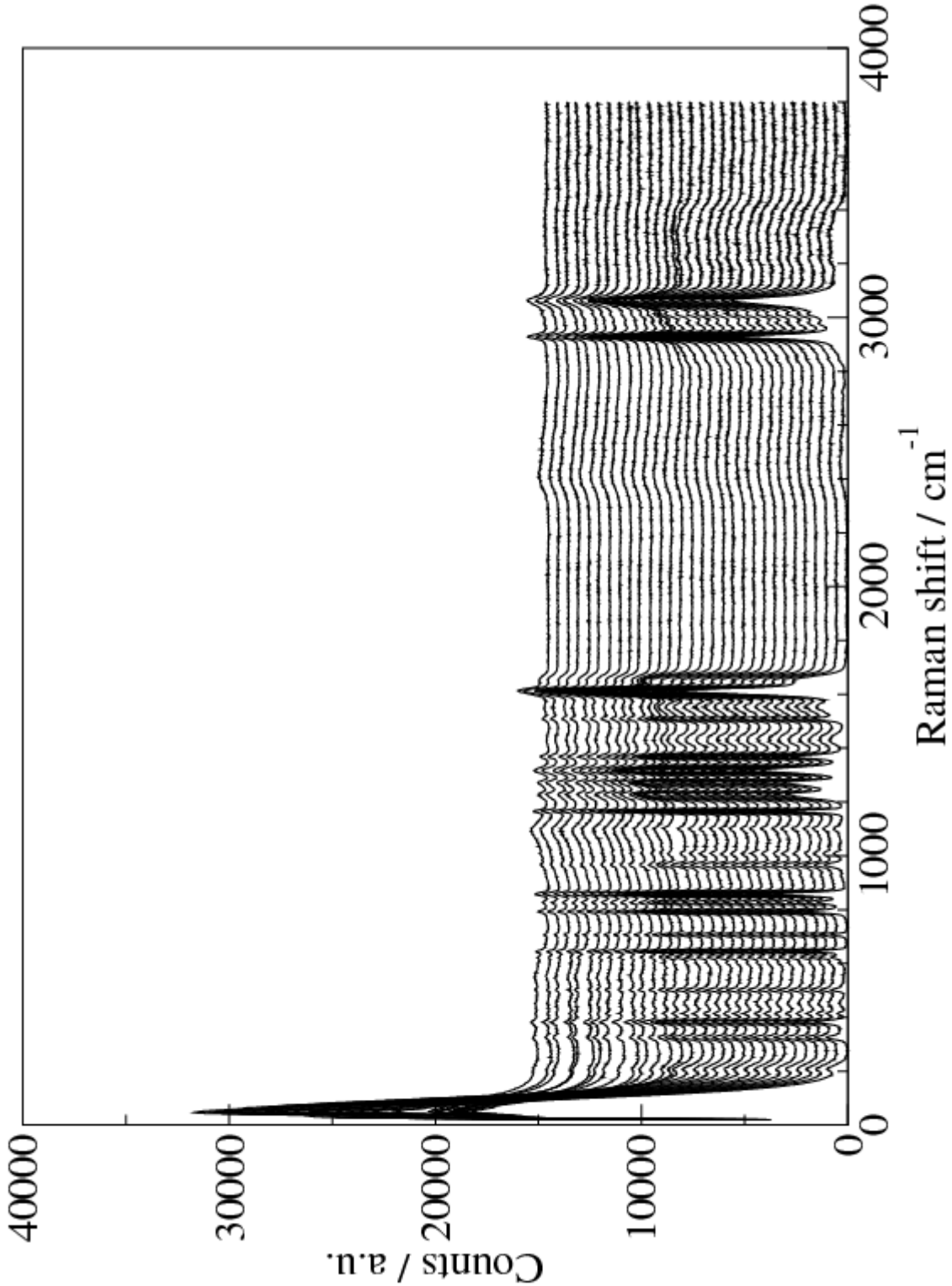

Figure S2a: 20 to 49 ° C (temperature increases in 1 ° C increments on moving vertically up the plot). Spectra are offset for clarity. A change in the spectra (assigned as the glass transition) occurs around 35 ° C.

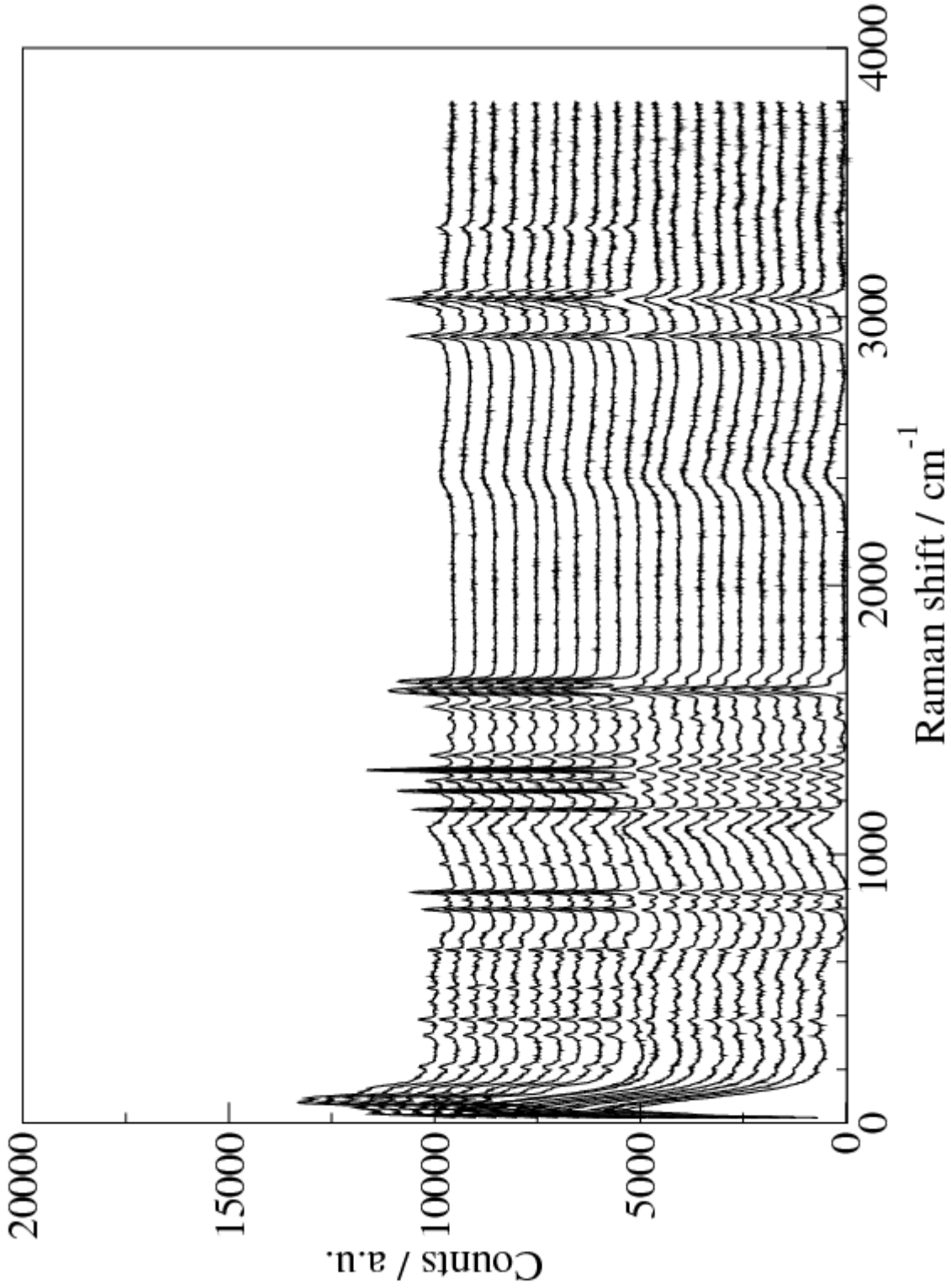

Figure S2b: 60 to 79 ° C (temperature increases in 1 ° C increments on moving vertically up the plot). Spectra are offset for clarity. This temperature range includes the crystallisation of the supercooled liquid to form III at 69–70 ° C.

Pa

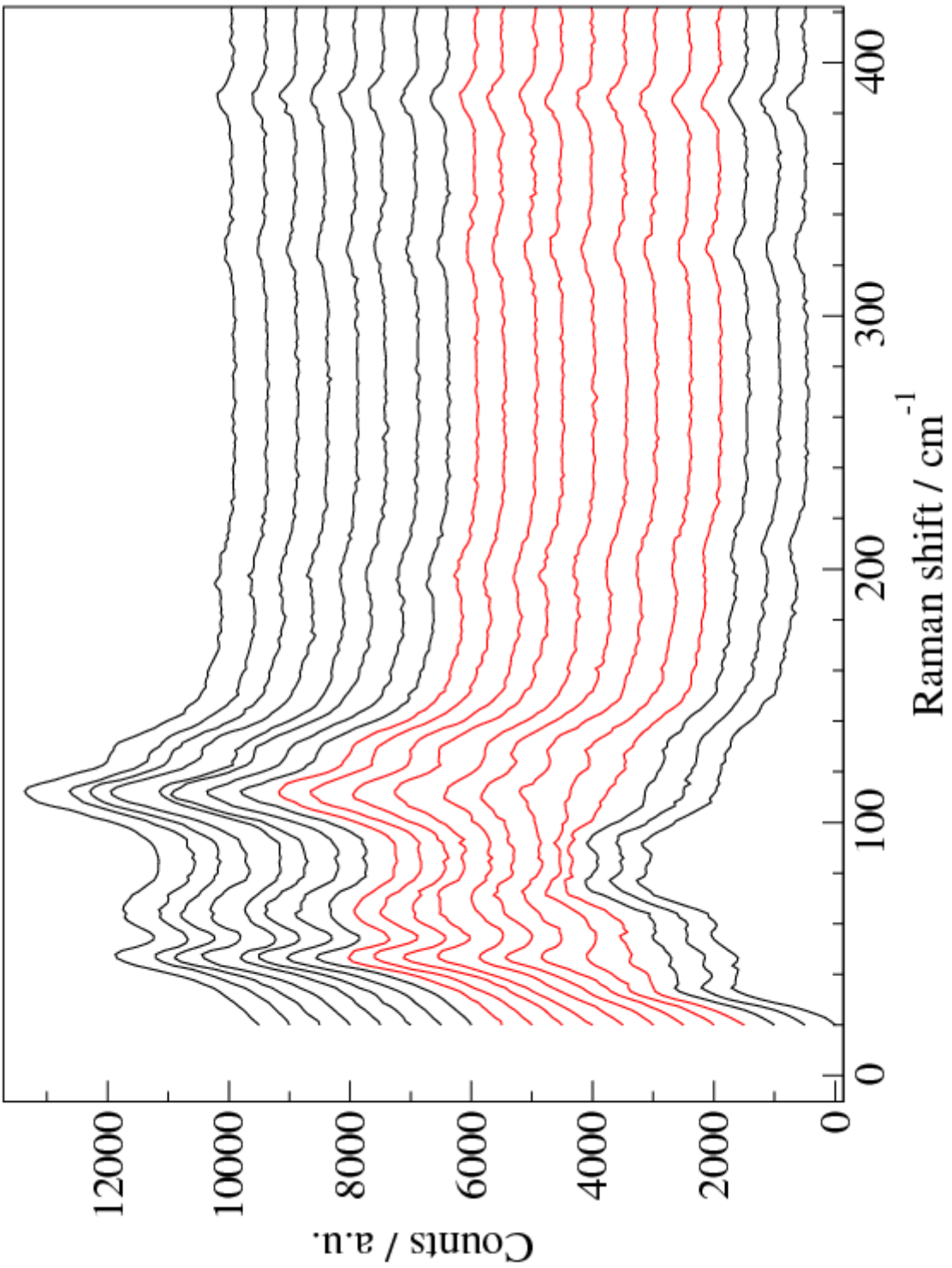

Figure S2c: 110 to 129 ° C (temperature increases in 1 ° C increments on moving vertically up the plot). Spectra are offset for clarity. These spectra cover the transformation from form III to form II at 110–120 ° C, which is highlighted in red. Phonon–mode data only are shown for this transformation.

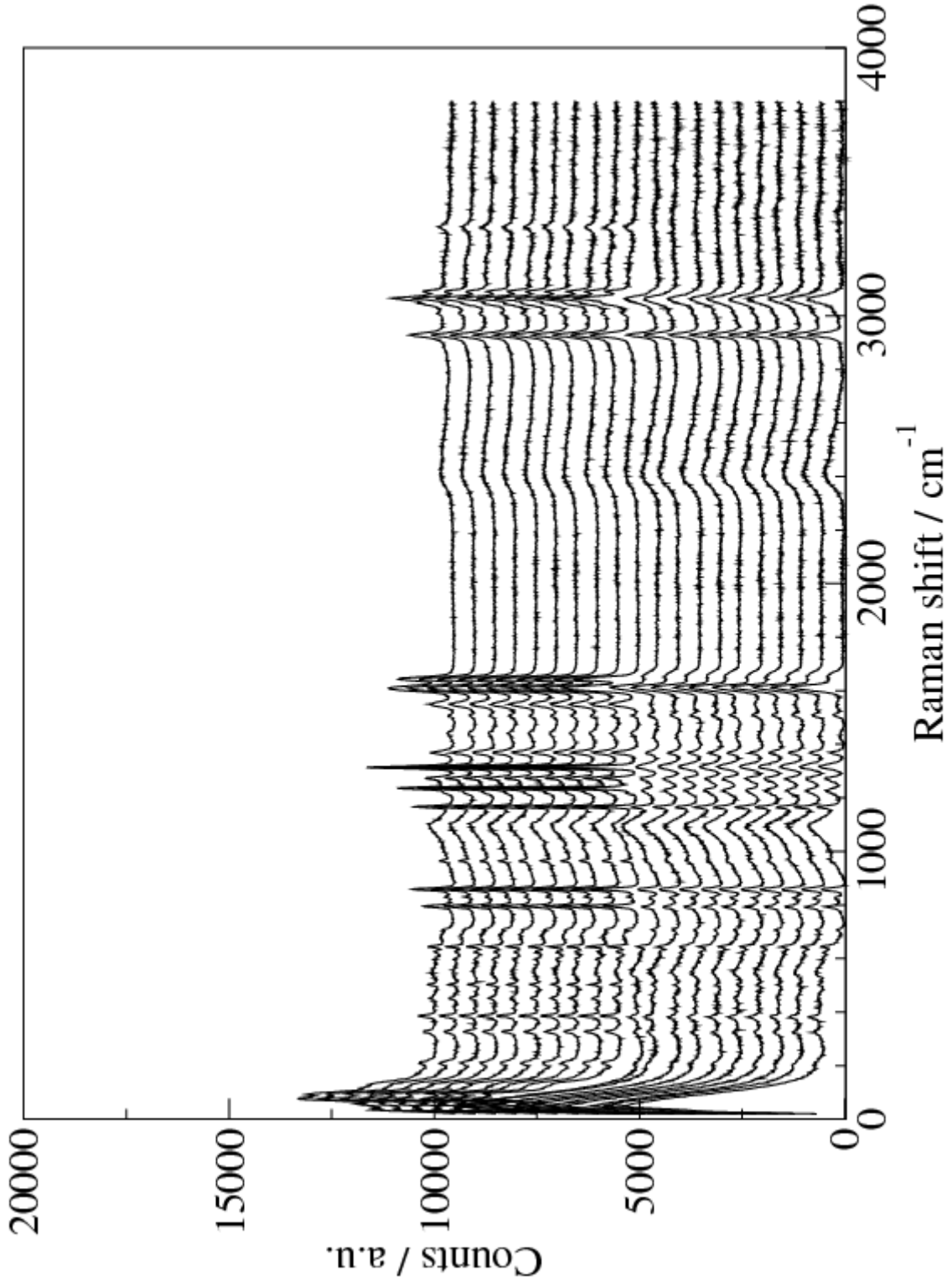

Figure S2d: 130 to 149 ° C (temperature increases in 1 ° C increments on moving vertically up the plot). Spectra are offset for clarity. These spectra cover the transformation from form II to form I at 139–140 ° C.

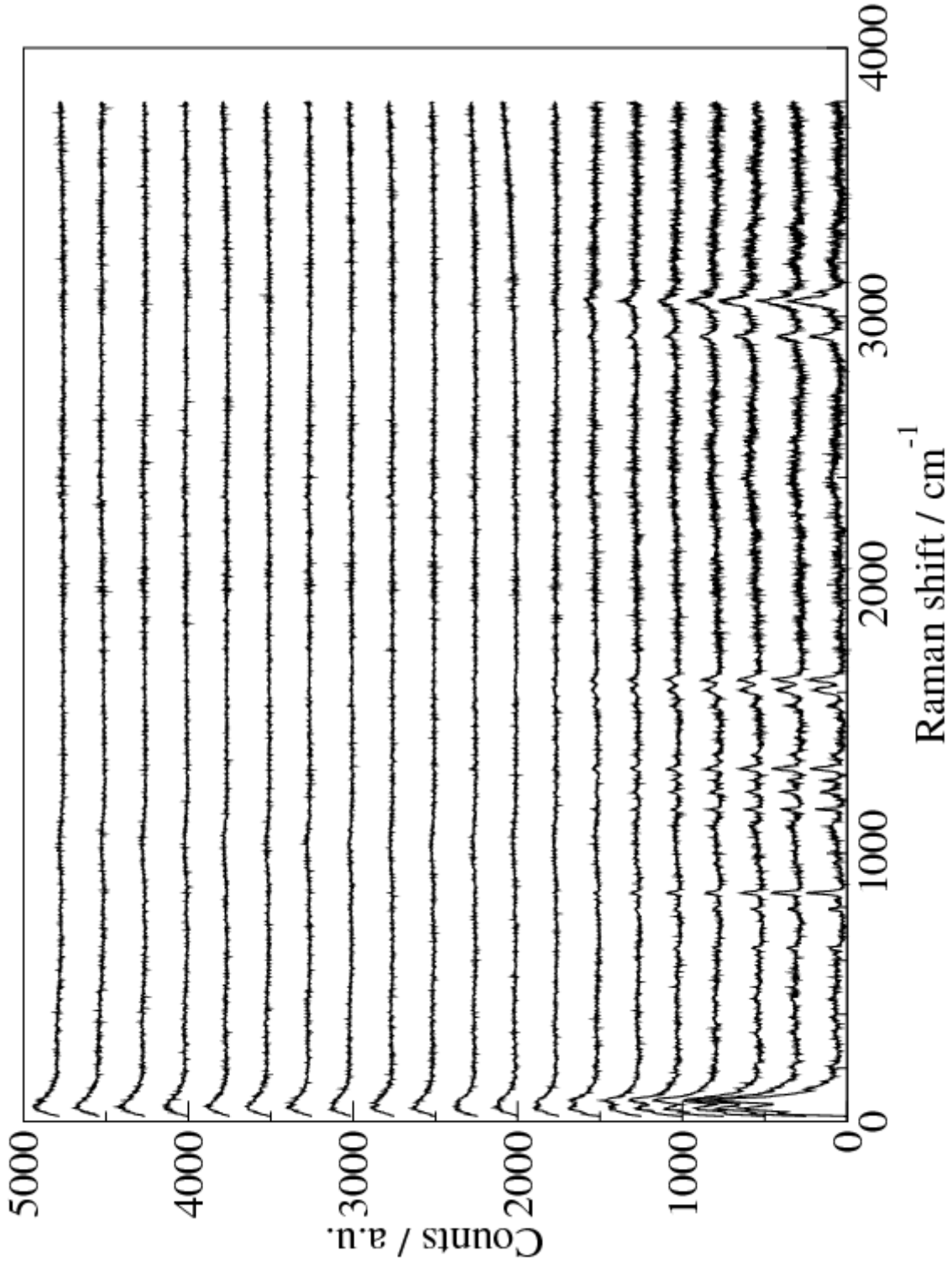

Figure S2e: 160 to 179 ° C (temperature increases in 1 ° C increments on moving vertically up the plot). Spectra are offset for clarity. These spectra cover the melting of form I (m/pt = 169 ° C).

Figure S3: Plot of scaled spectra at various temperatures. This figure can be compared directly with Figure 3 in the publication of Kauffman et al [29], from which it can be seen that by 154 ° C our experiment has yielded form I, whereas Kauffman's sample remained as form II.

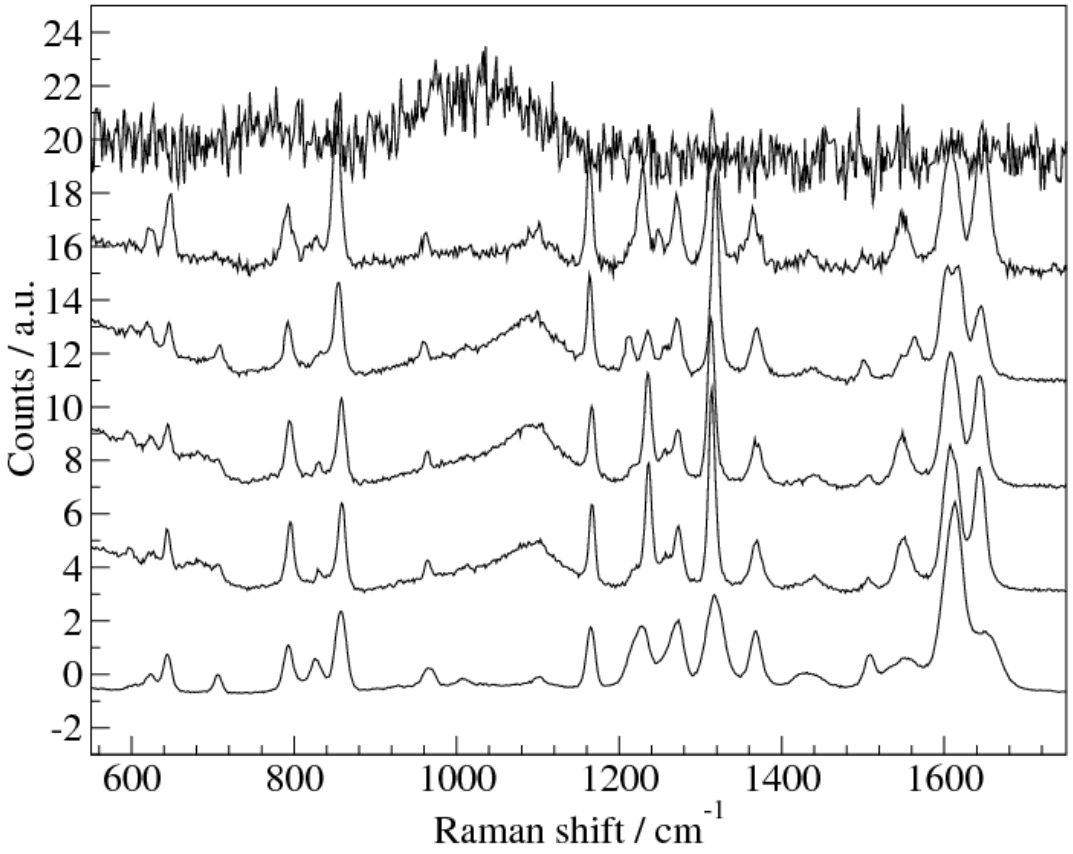

Figure S3: Spectra collected at: 25, 72, 101, 130, 154, 175 ° C (temperature increases on moving vertically up the plot, spectra are scaled and offset for clarity).

Figure S4: PCA of selected spectra regions: a) 1450–1700 cm^{-1}; b) 2800–3200 cm^{-1}.

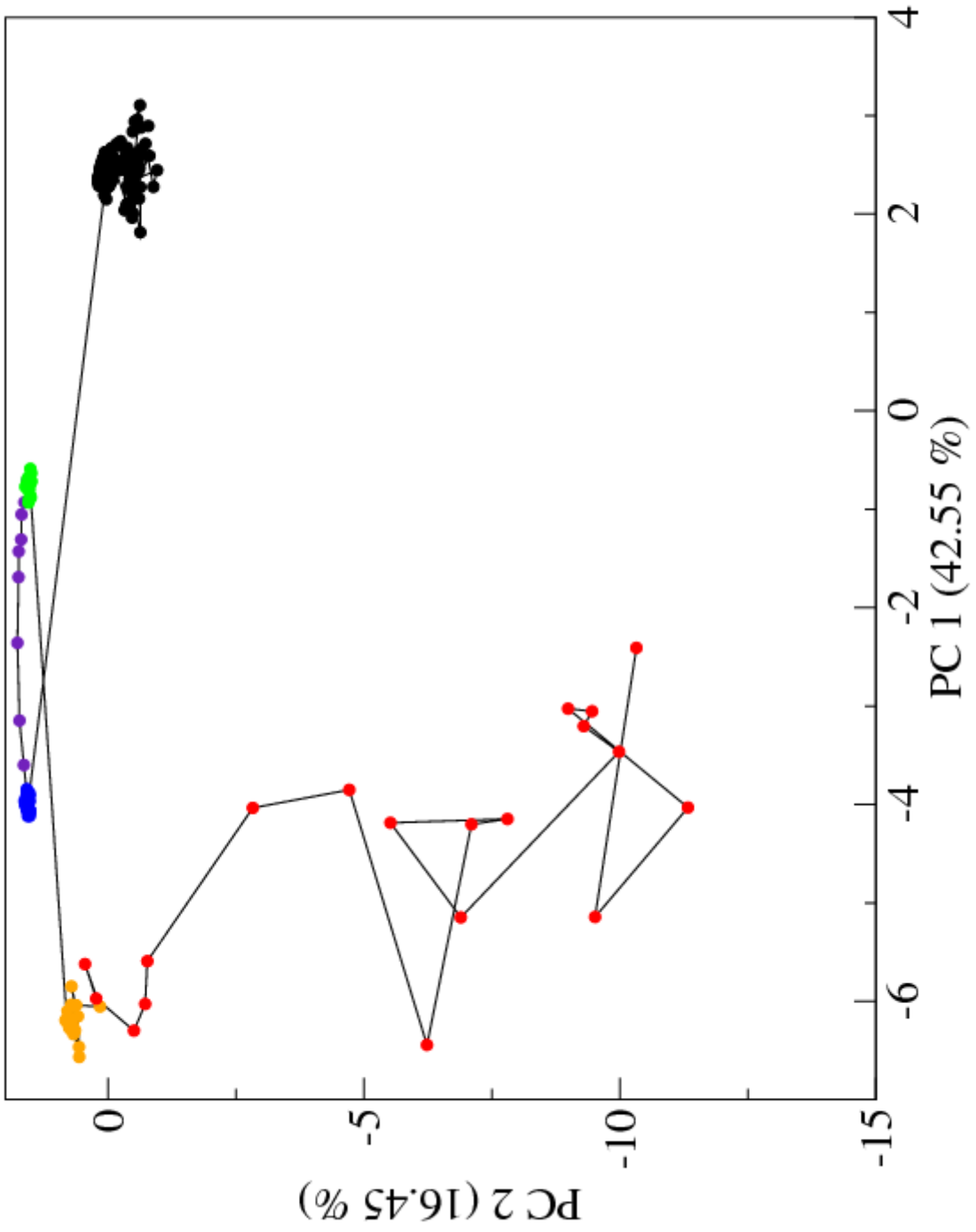

Figure S4a: Scores plot for scaled data in spectral window 1450–1750 cm^{-1}. Colours are as per Figure 2.

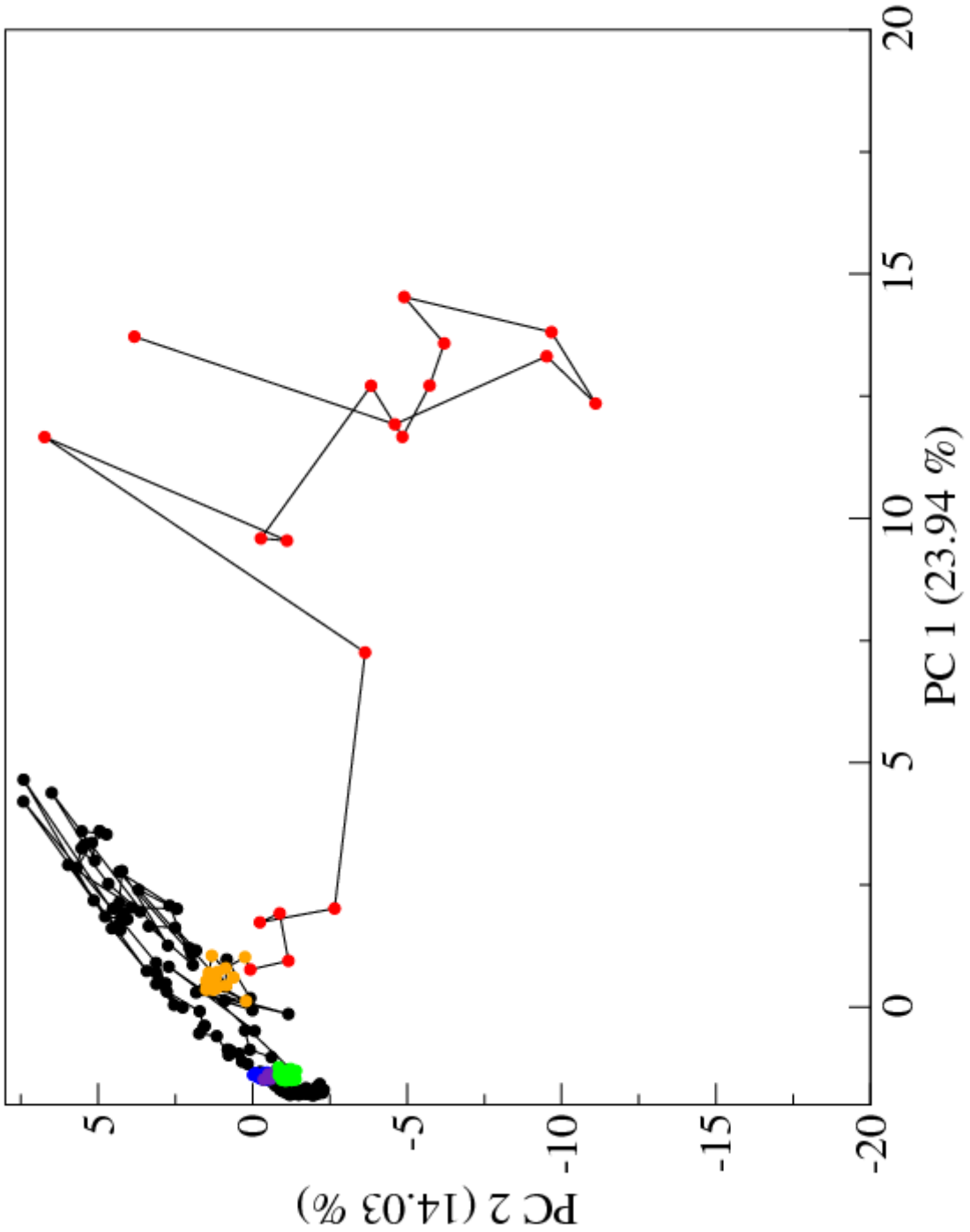

Figure S4b: Scores plot for scaled data in spectral window 2800–3200 cm^{-1}. Colours are as per Figure 2.