# SUPPORTING INFORMATION

## Thermal behavior of the potassium $C_1$-$C_{12}$ *n*-alkanoates and its relevance to Fischer–Tropsch

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The primary aim of the investigation was to study the thermal behavior of the potassium $C_1$-$C_{12}$ *n*-alkanoates (K-carboxylates). The spectroscopic data was collected and employed to support the thermal investigation.

(a) *Thermal analyses*. Only a single example of the calorigram of each compound recorded by differential scanning calorimetry (DSC) is presented (Figures S1 to S12), even though each compound was analyzed multiple times and with temperature programs. The outcome of the thermal analyses is documented in detail in the main manuscript. One set of thermogravimetric analysis data is also included (Figure S13).

(b) *Infrared spectroscopy* (IR). The IR spectrum is sensitive for the detection of carbonyl and carboxylate compounds. It could therefore be used to confirm synthesis of the potassium carboxylates, as well as provide an indication of purity. Syntheses were performed with a 2 % molar excess of carboxylic acid. If the carboxylic acid was not completely removed during the purification step, it would be visible on the infrared spectrum.

IR spectroscopy was also employed to determine whether chemical changes took place during calorimetry. Once a thermal event was observed, a sample was run to a temperature just above the temperature of the observed thermal event and the IR spectrum of the sample thus treated was collected and compared with the starting material. Representative IR spectra are presented (Figures S14 to S25). The temperature indicated in association with an IR spectrum refers to the temperature to which the sample was heated. All spectra were recorded at ambient conditions.

The spectra were recorded with a diamond attenuated total reflectance (ATR) attachment. The absorption in the wave number region $\nu/\mathrm{cm}^{-1}$ = (550 to 500) is due to this method of analysis.

(c) *Raman spectroscopy*. The Raman spectra were collected (Figures S26 to S37) to support interpretation of the IR spectra. However, it was found that the K-carboxylates, unlike the Li-carboxylates investigated previously (*J. Chem. Eng. Data* **2013**, *58*, 1039-1049), were not present in two spectroscopically different configurations. A single pair of carboxylate stretching vibrations was observed and in the manuscript little discussion was devoted to spectroscopy.

(d) *UV-Visible spectroscopy* (UV-vis). Although no specific additional information was anticipated from the UV-vis spectra, these spectra were collected (Figures S38 to S49) as a matter of routine.

## 1. Differential Scanning Calorimetry

### *1.1. Potassium Methanoate*

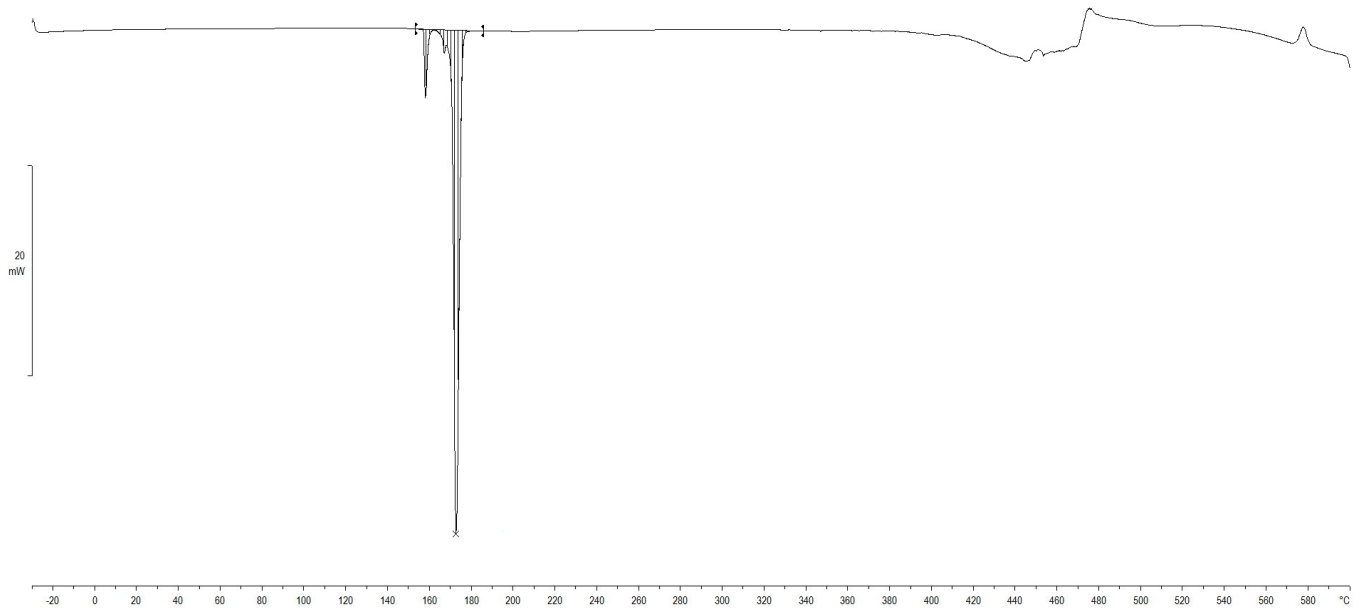


**Figure S1.** Calorigram of potassium methanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

### *1.2. Potassium Ethanoate*

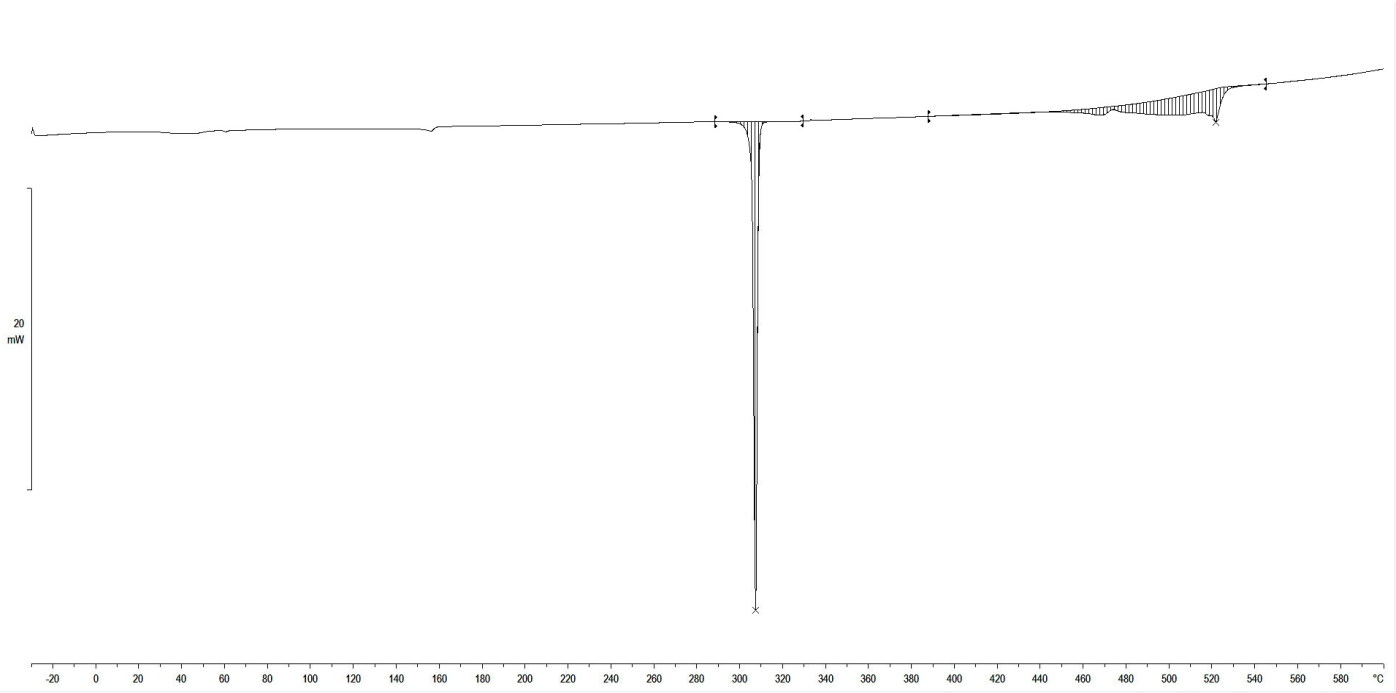


**Figure S2.** Calorigram of potassium ethanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.3. Potassium Propanoate*

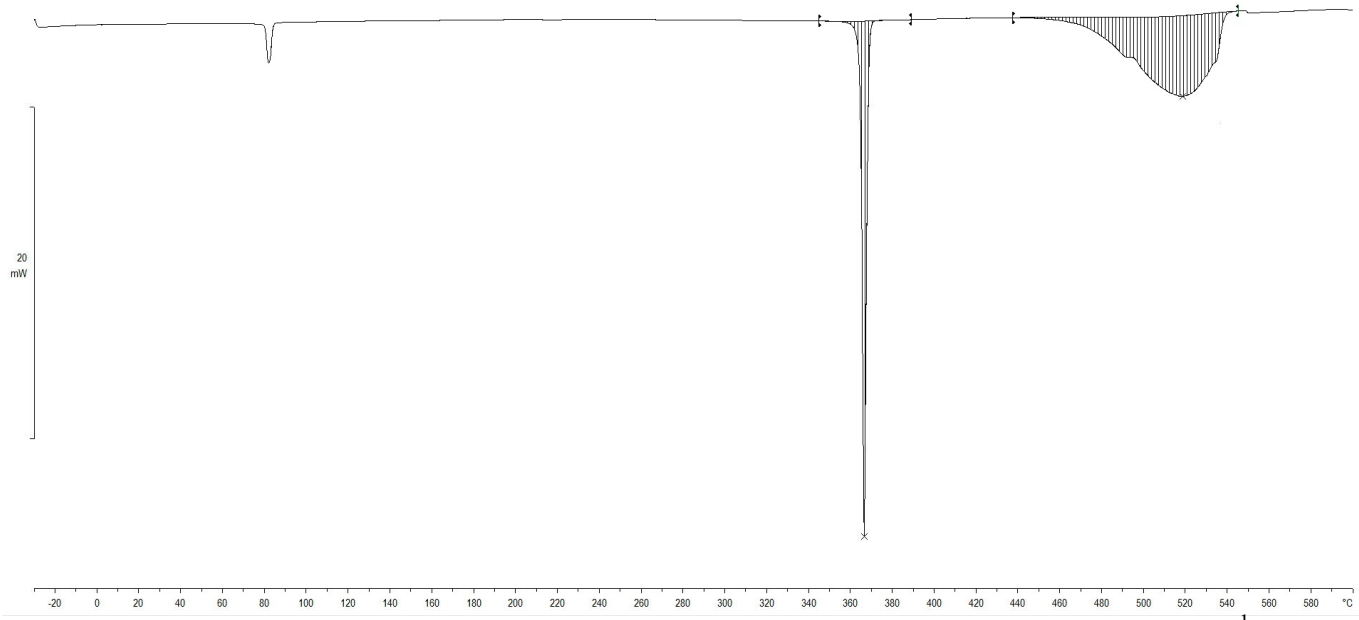


**Figure S3.** Calorigram of potassium propanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.4. Potassium Butanoate (butyrate)*

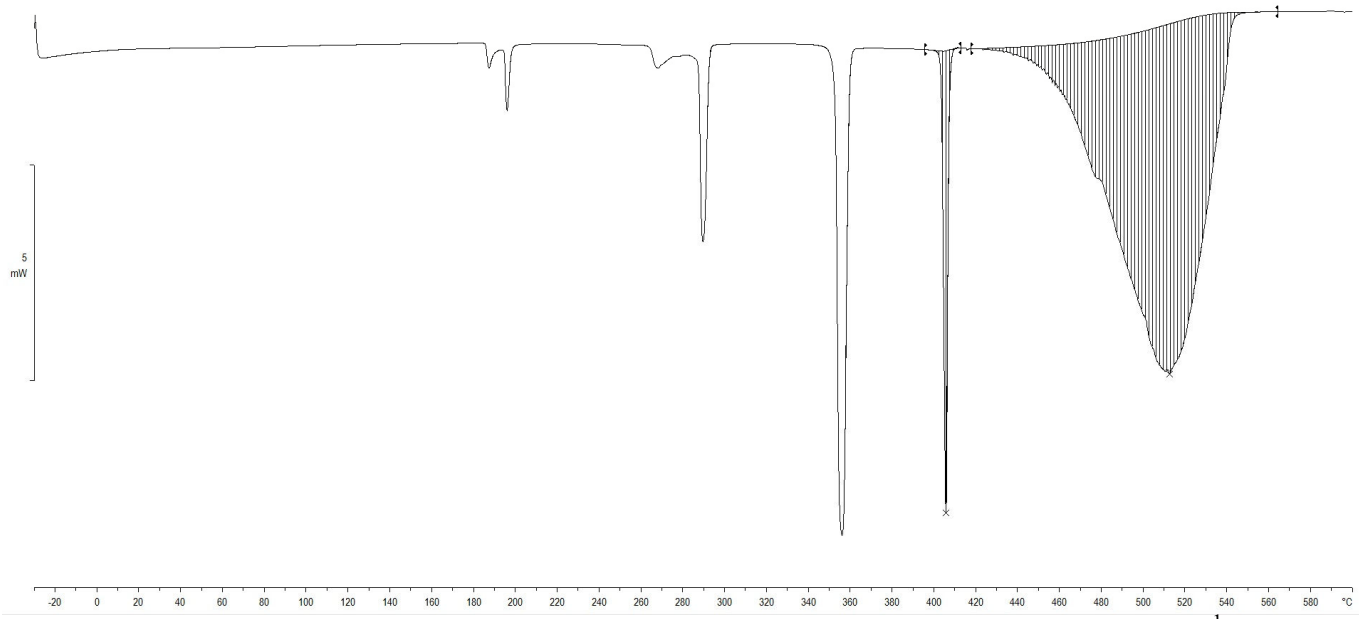


**Figure S4.** Calorigram of potassium butanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.5. Potassium Pentanoate (valerate)*

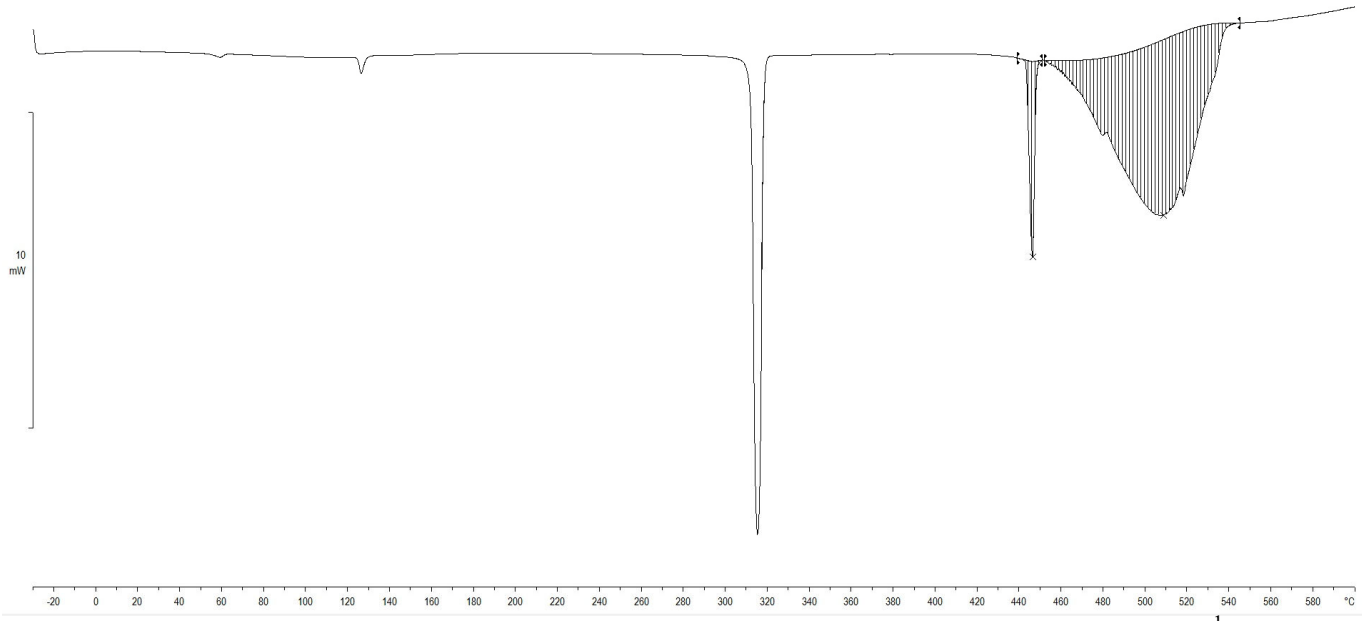


**Figure S5.** Calorigram of potassium pentanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.6. Potassium Hexanoate (caproate)*

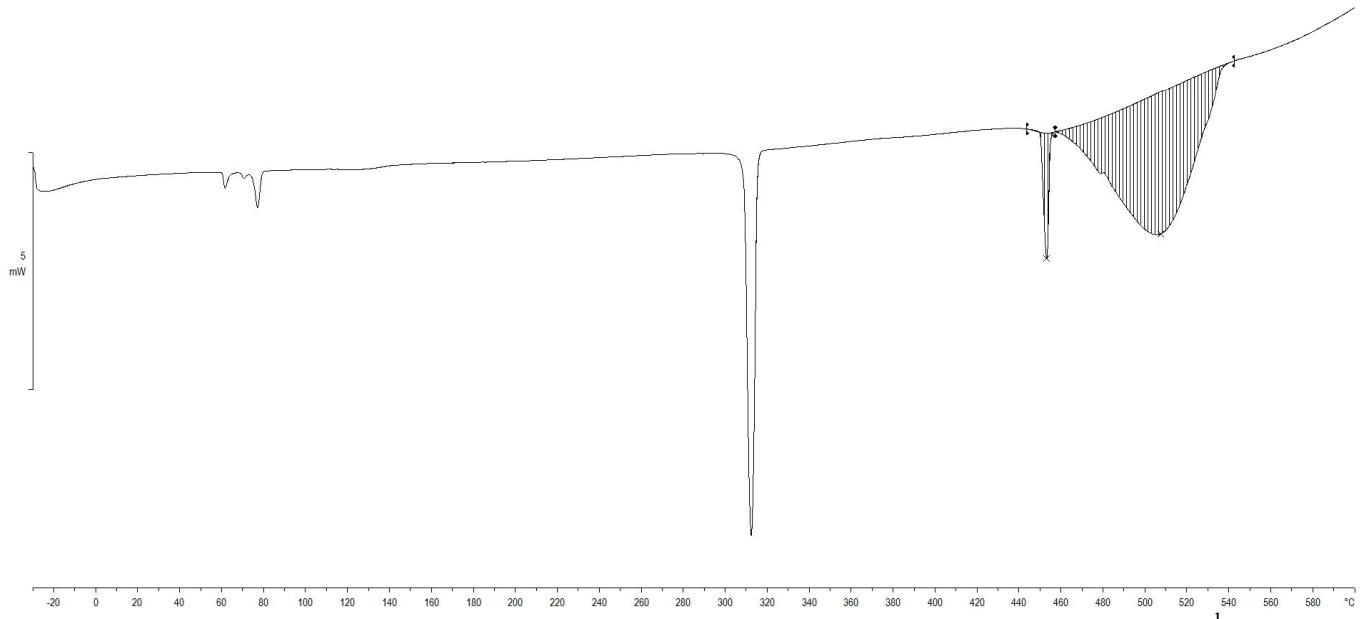


**Figure S6.** Calorigram of potassium hexanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.7. Potassium Heptanoate*

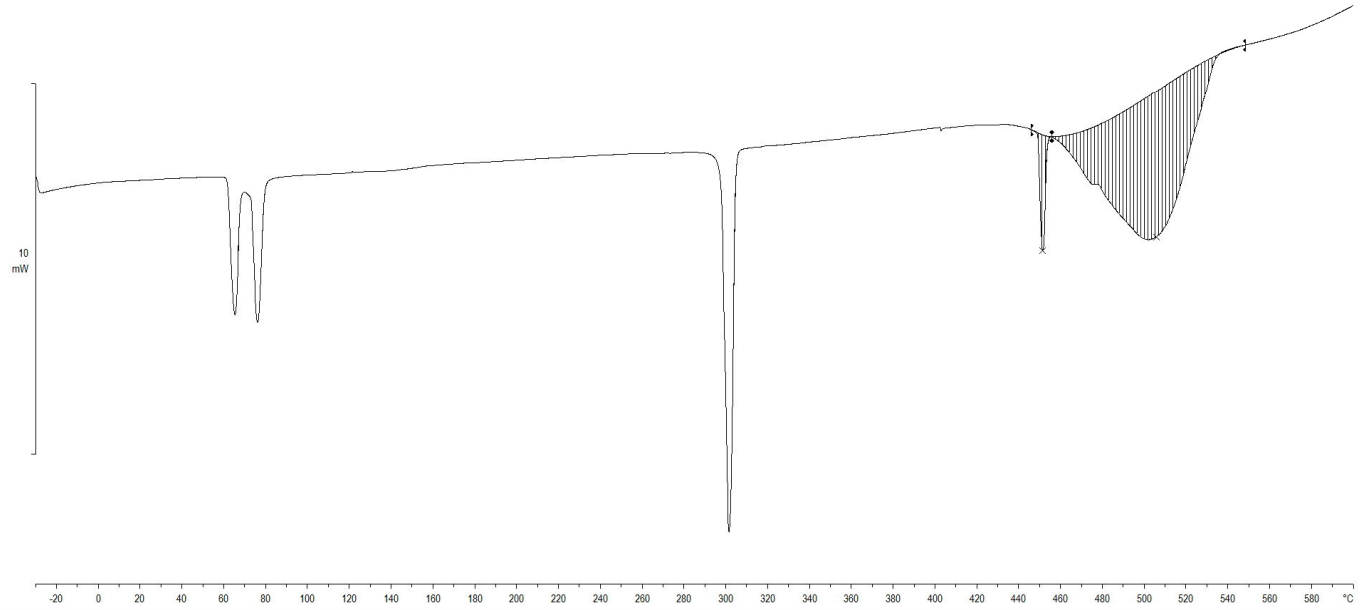


**Figure S7.** Calorigram of potassium heptanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.8. Potassium Octanoate (caprylate)*

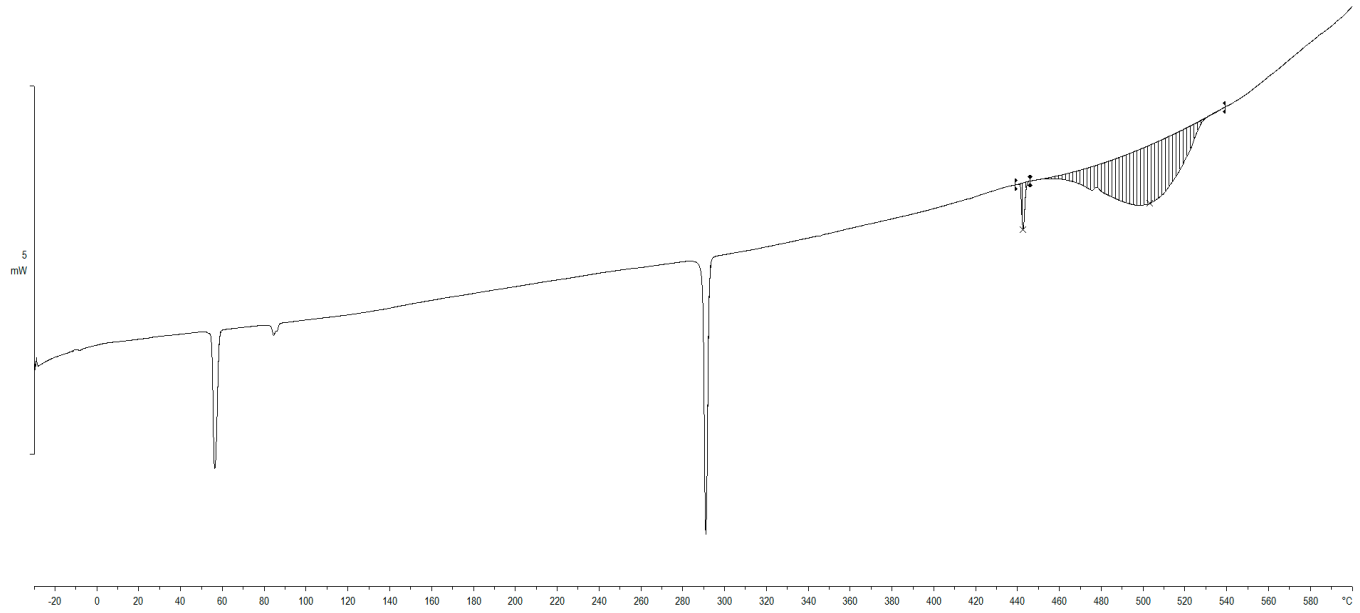


**Figure S8.** Calorigram of potassium octanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.9. Potassium Nonanoate (pelargonate)*

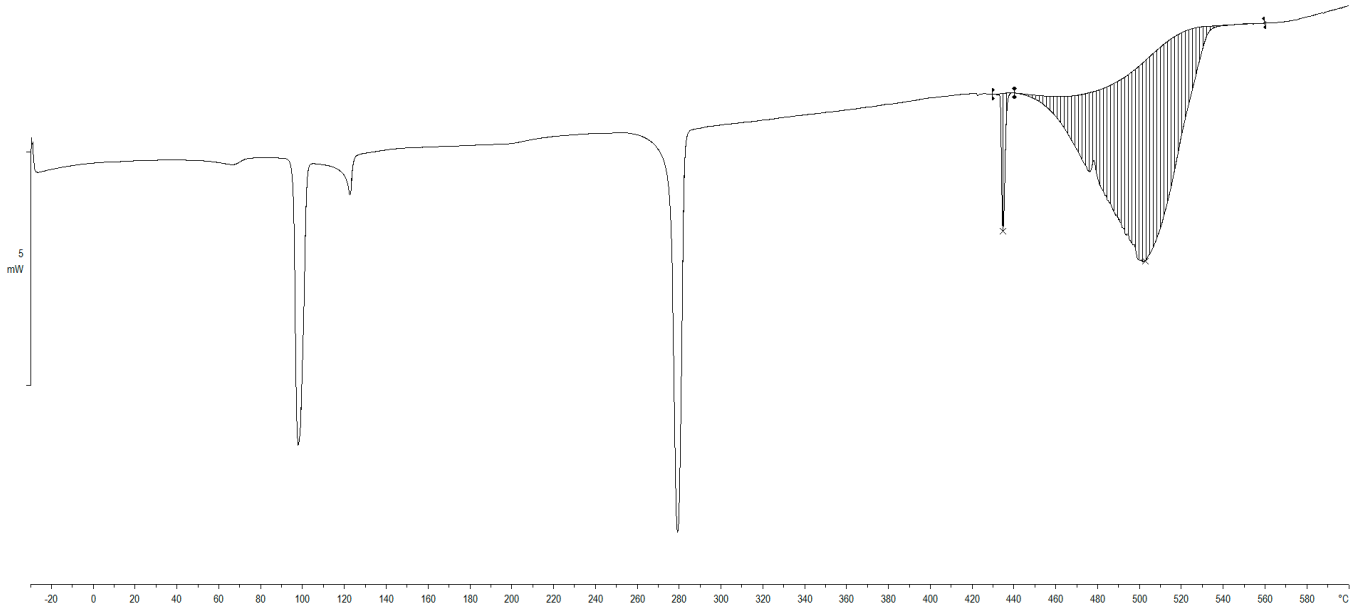


**Figure S9.** Calorigram of potassium nonanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.10. Potassium Decanoate (caprate)*

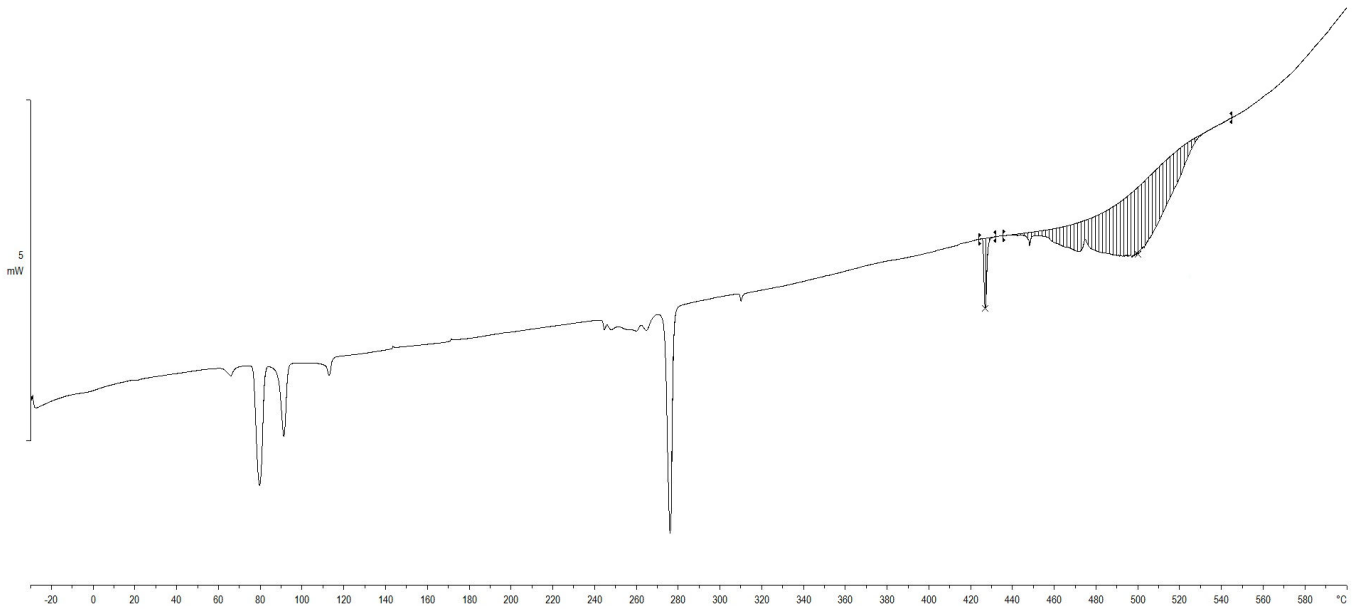


**Figure S10.** Calorigram of potassium decanoate over the range $t$/°C = (-30 to 600) with $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.11. Potassium Undecanoate*

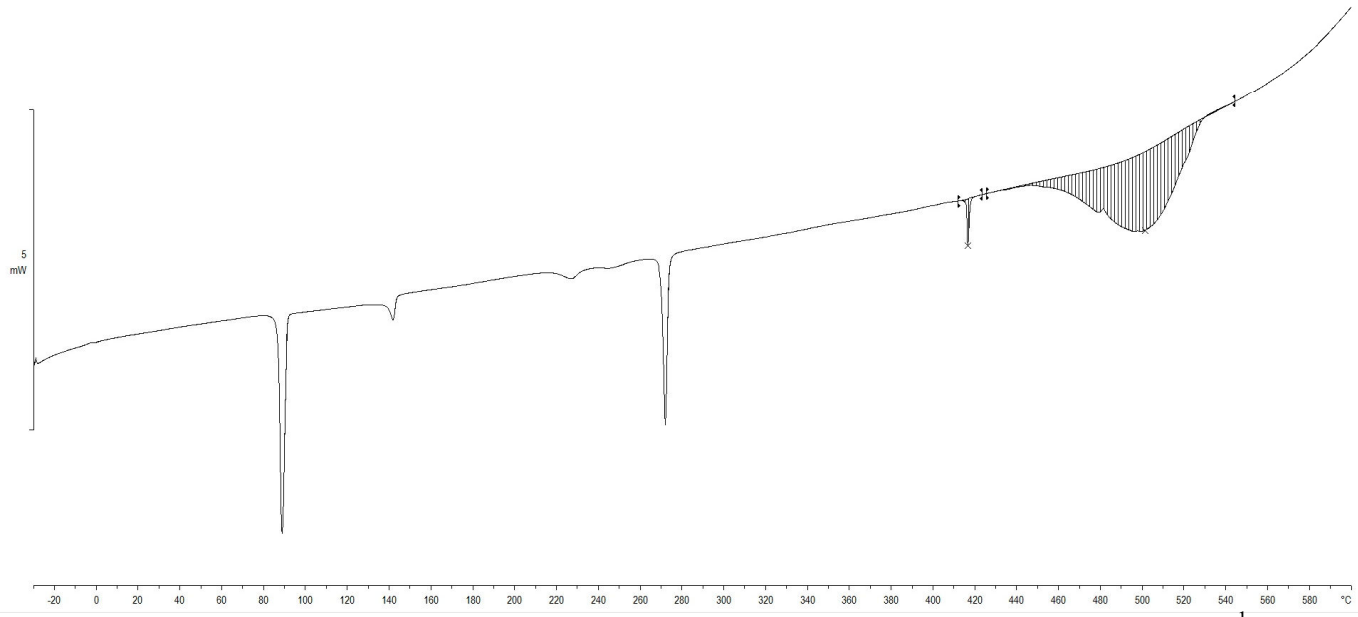


**Figure S11.** Calorigram of potassium undecanoate over the range $t$/°C = (-30 to 600) and $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

*1.12. Potassium Dodecanoate (laurate)*

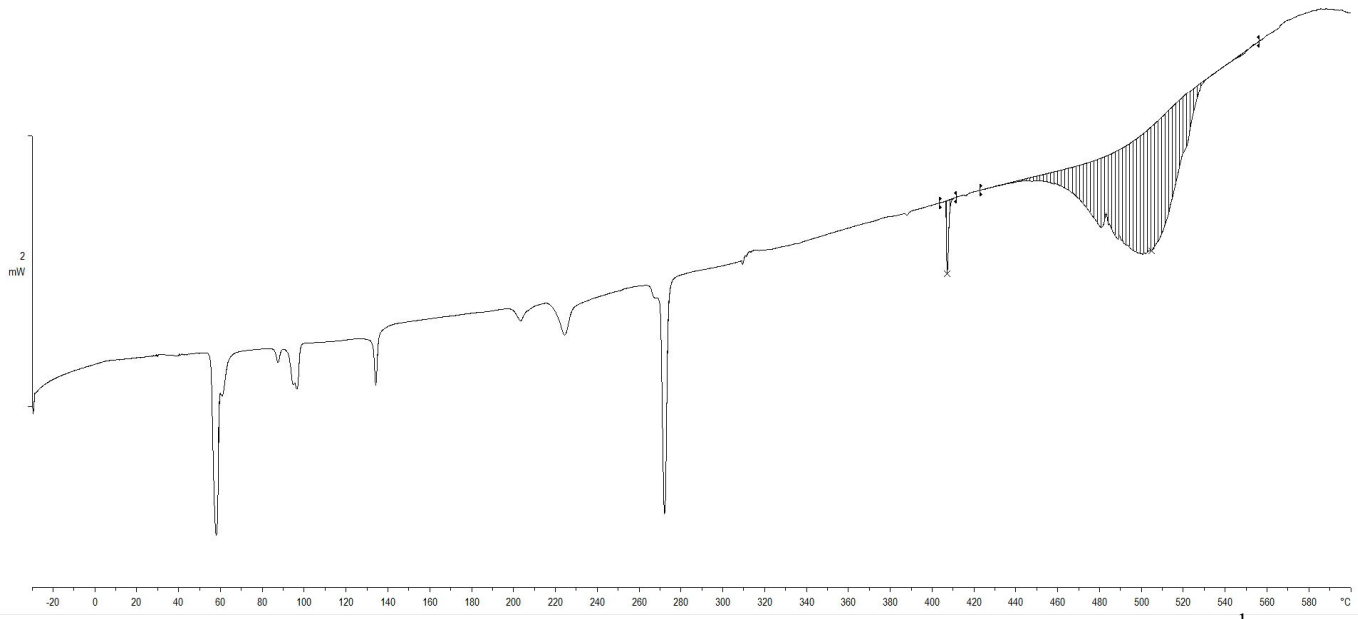


**Figure S12.** Calorigram of potassium dodecanoate over the range $t$/°C = (-30 to 600) and $\beta$/°C·s$^{-1}$ = (0.167) under $N_2$ inert atmosphere.

## 2. Thermogravimetric analysis

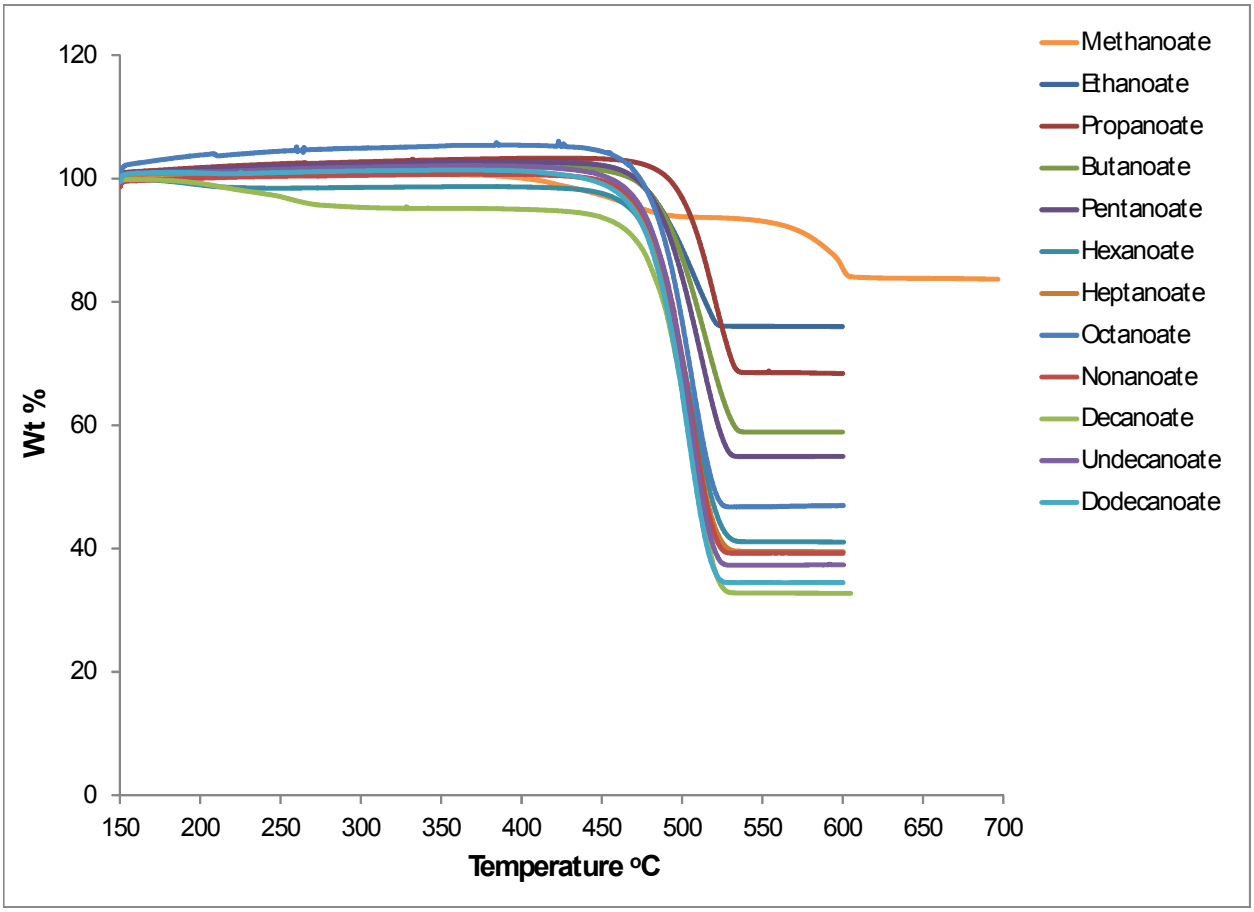


**Figure S13.** Mass loss versus temperature profiles of the potassium $C_1$-$C_{12}$ *n*-alkanoates over the temperature range *t*/°C = (150 to 600) and in the case of potassium methanoate over the range *t*/°C = (150 to 700).

## 3. Infrared spectroscopy

### *3.1. Potassium methanoate (formate)*

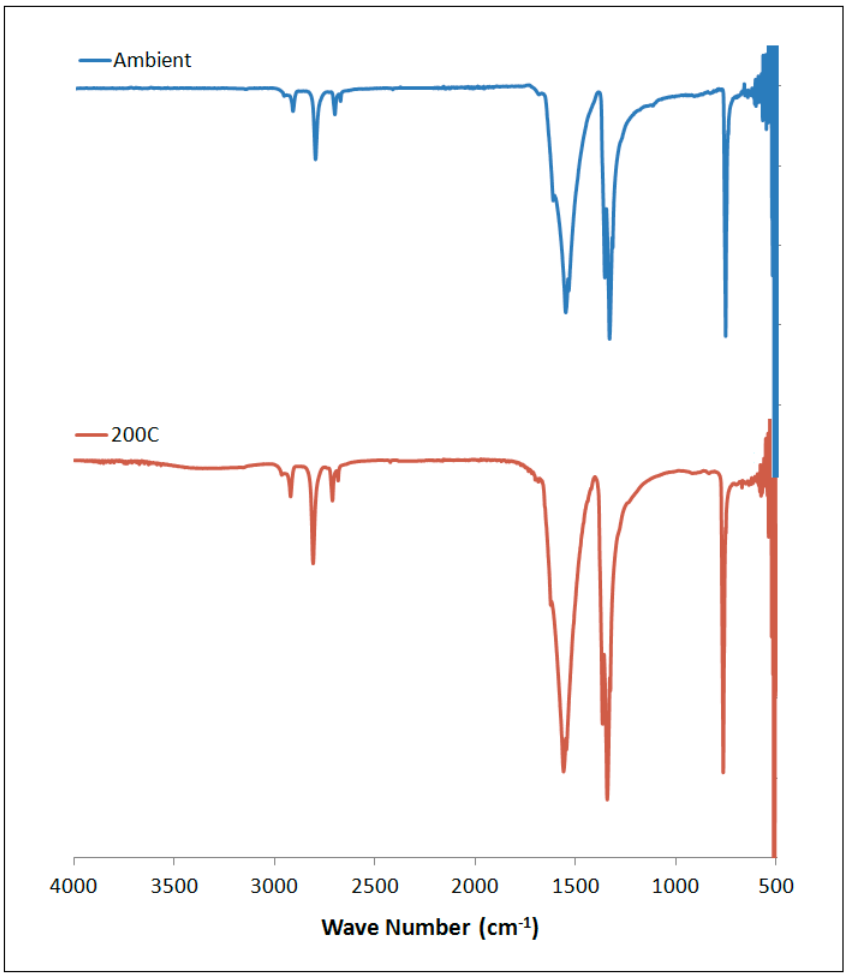


**Figure S14.** IR spectra of potassium methanoate collected over the wave number region $\nu$/cm$^{-1}$ = (4000 to 500) before and after melting.

*3.2. Potassium ethanoate (acetate)*

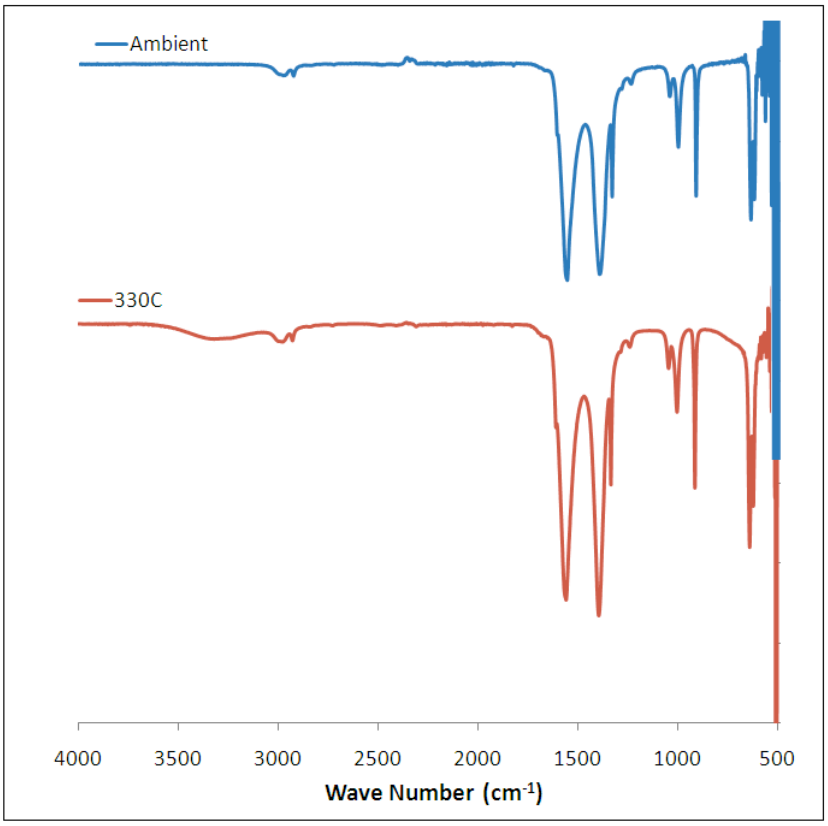


**Figure S15.** IR spectra of potassium ethanoate collected over the wave number region $\nu/cm^{-1}$ = (4000 to 500) before and after melting.

### 3.3. *Potassium propanoate*

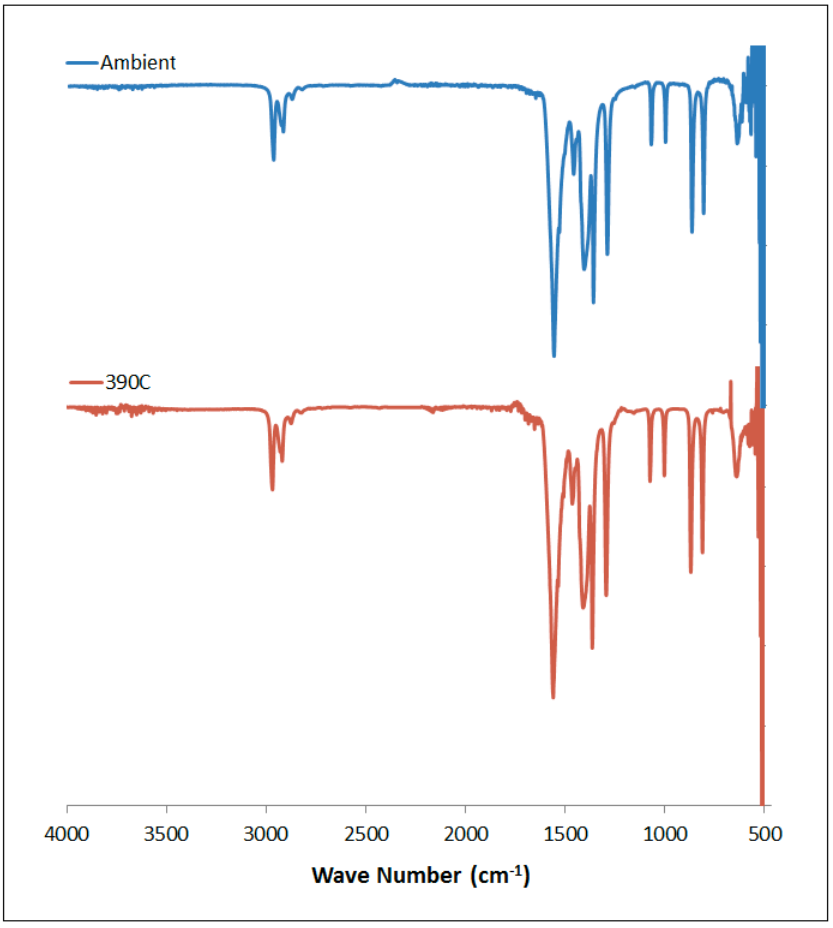


**Figure S16.** IR spectra of potassium propanoate collected over the wave number region $\tilde{\nu}/cm^{-1}$ = (4000 to 500) before and after melting.

*3.4. Potassium butanoate (butyrate)*

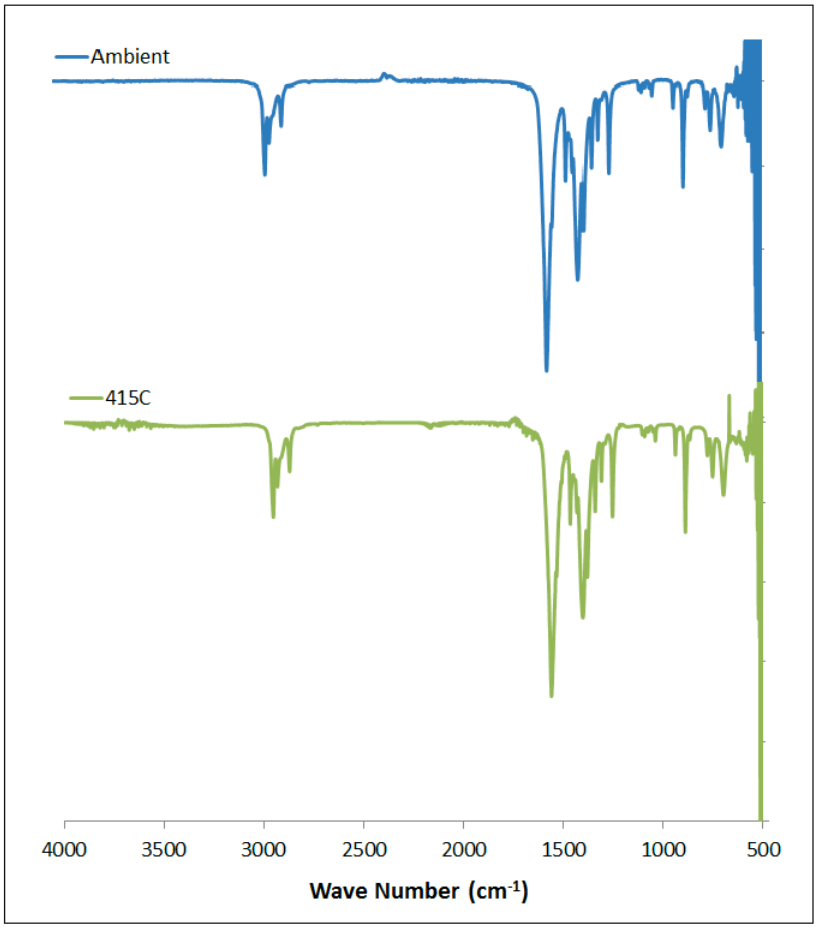


**Figure S17.** IR spectra of potassium butanoate collected over the wave number region $\nu/cm^{-1}$ = (4000 to 500) before and after melting.

*3.5. Potassium pentanoate (valerate)*

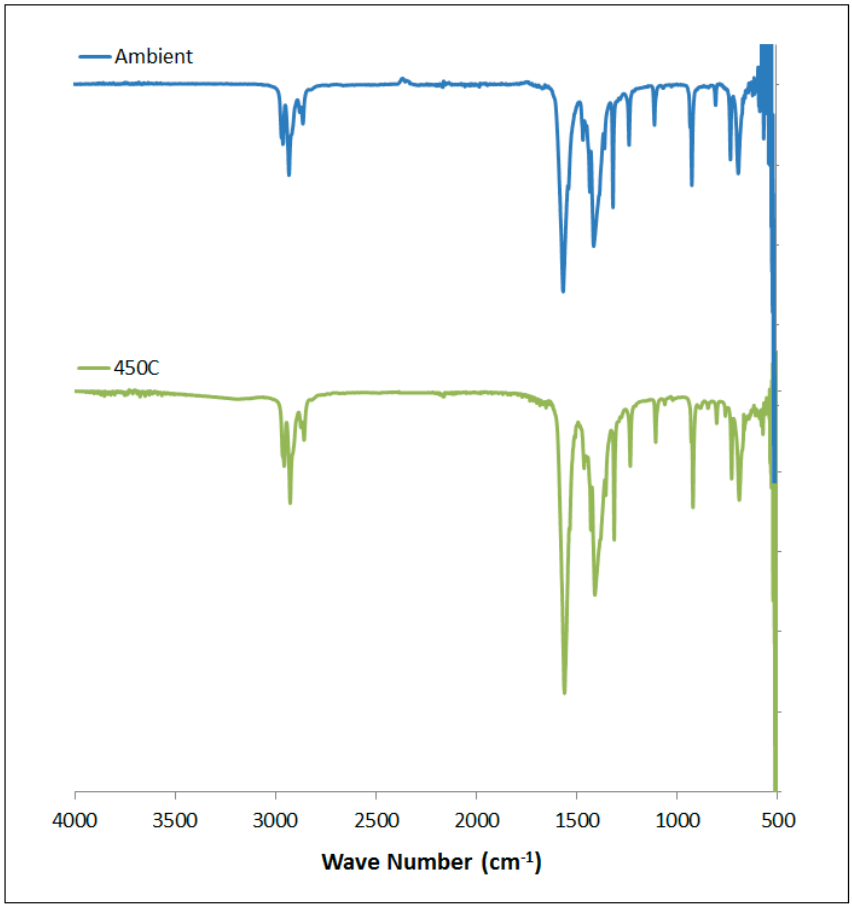


**Figure S18.** IR spectra of potassium pentanoate collected over the wave number region $\nu/cm^{-1}$ = (4000 to 500) before and after melting.

*3.6. Potassium hexanoate (caproate)*

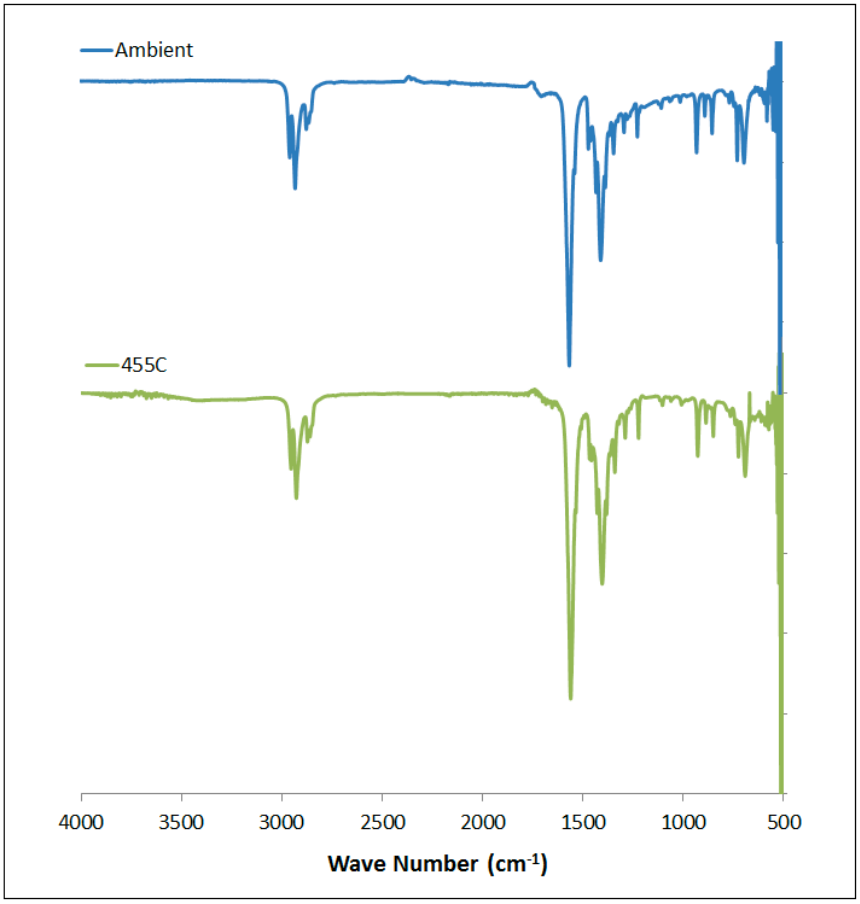


**Figure S19.** IR spectra of potassium hexanoate collected over the wave number region $\tilde{\nu}/cm^{-1}$ = (4000 to 500) before and after melting.

*3.7. Potassium heptanoate*

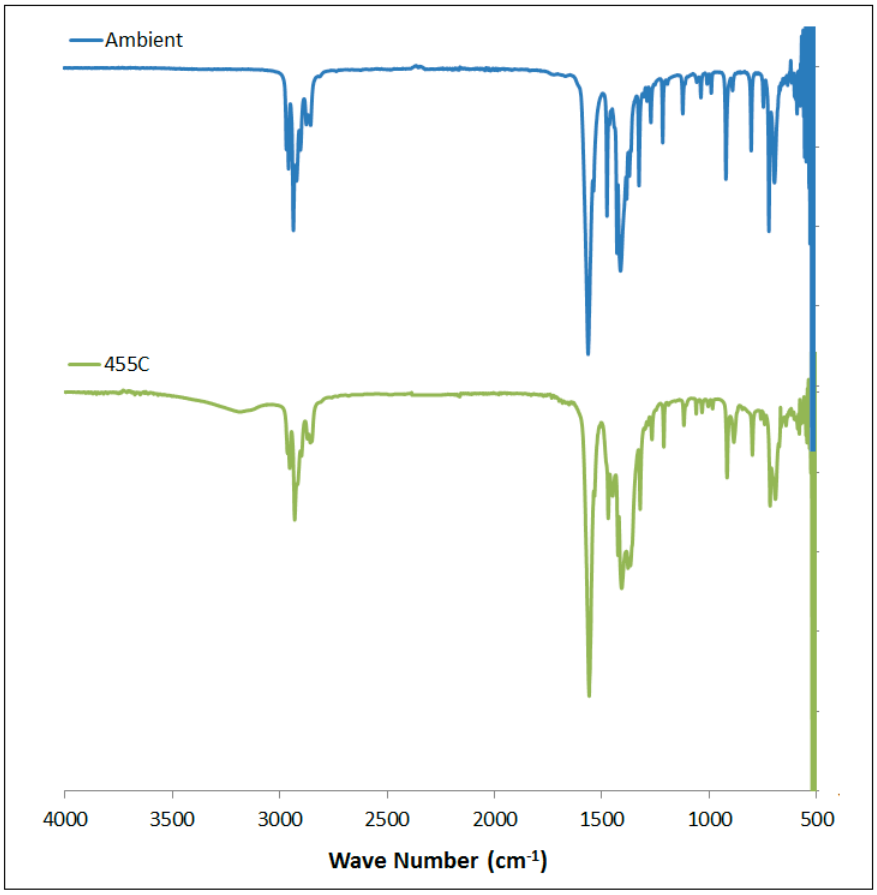


**Figure S20.** IR spectra of potassium heptanoate collected over the wave number region $\nu/cm^{-1}$ = (4000 to 500) before and after melting.

*3.8. Potassium octanoate (caprylate)*

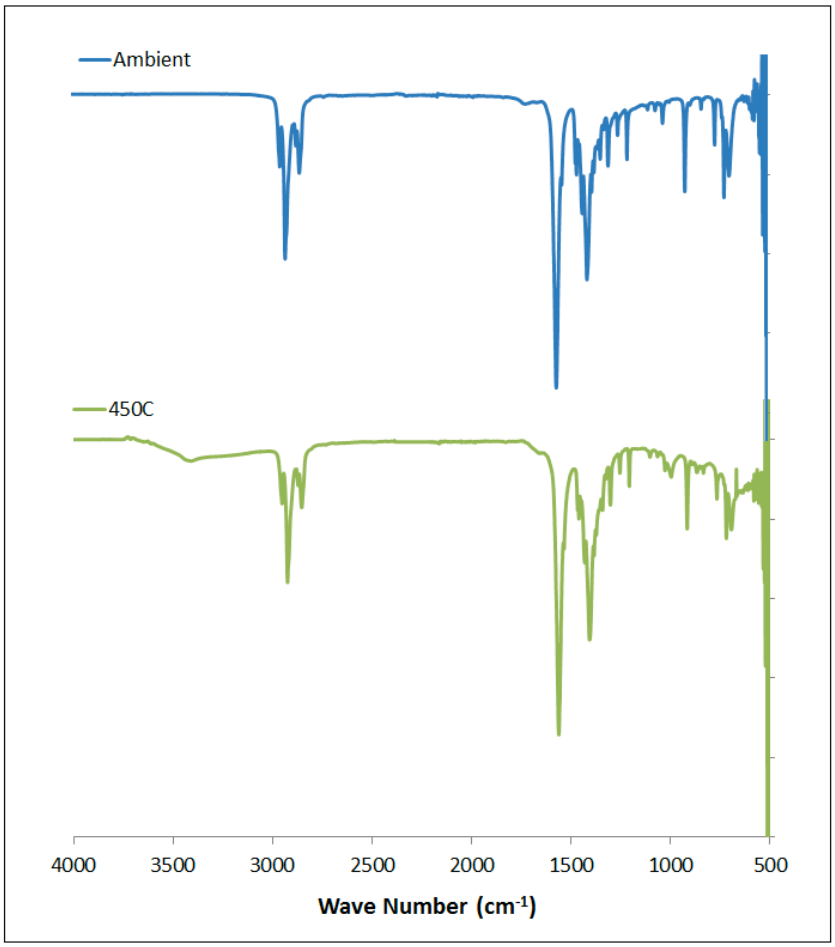


**Figure S21.** IR spectra of potassium octanoate collected over the wave number region $\tilde{\nu}/cm^{-1}$ = (4000 to 500) before and after melting.

*3.9. Potassium nonanoate (pelargonate)*

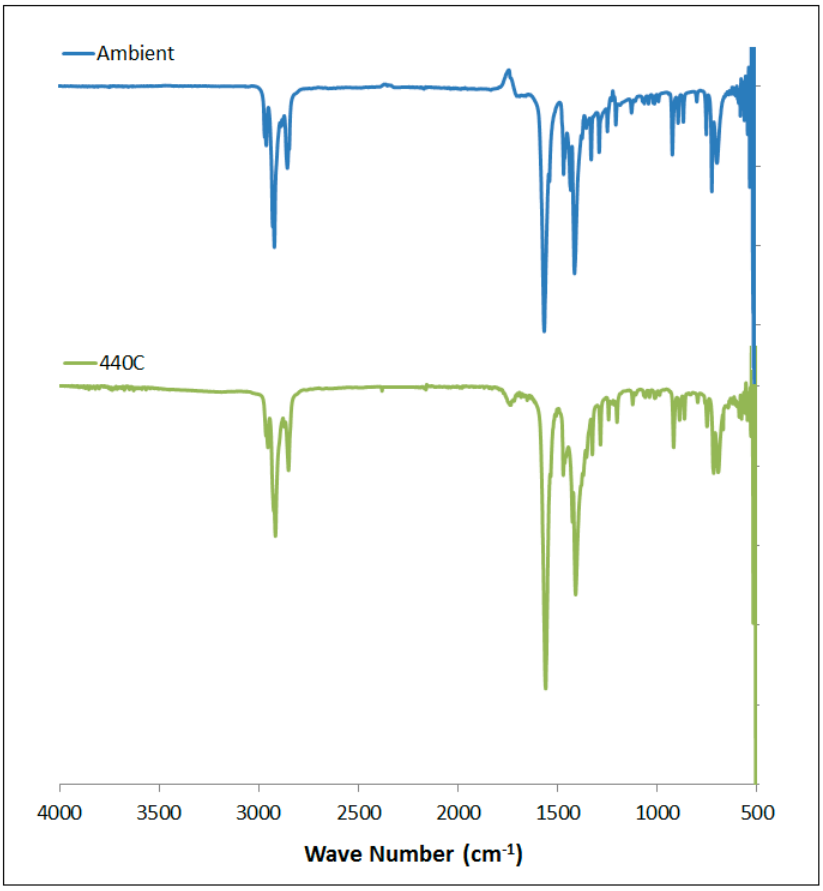


**Figure S22.** IR spectra of potassium nonanoate collected over the wave number region $\nu/cm^{-1}$ = (4000 to 500) before and after melting.

*3.10. Potassium decanoate (caprate)*

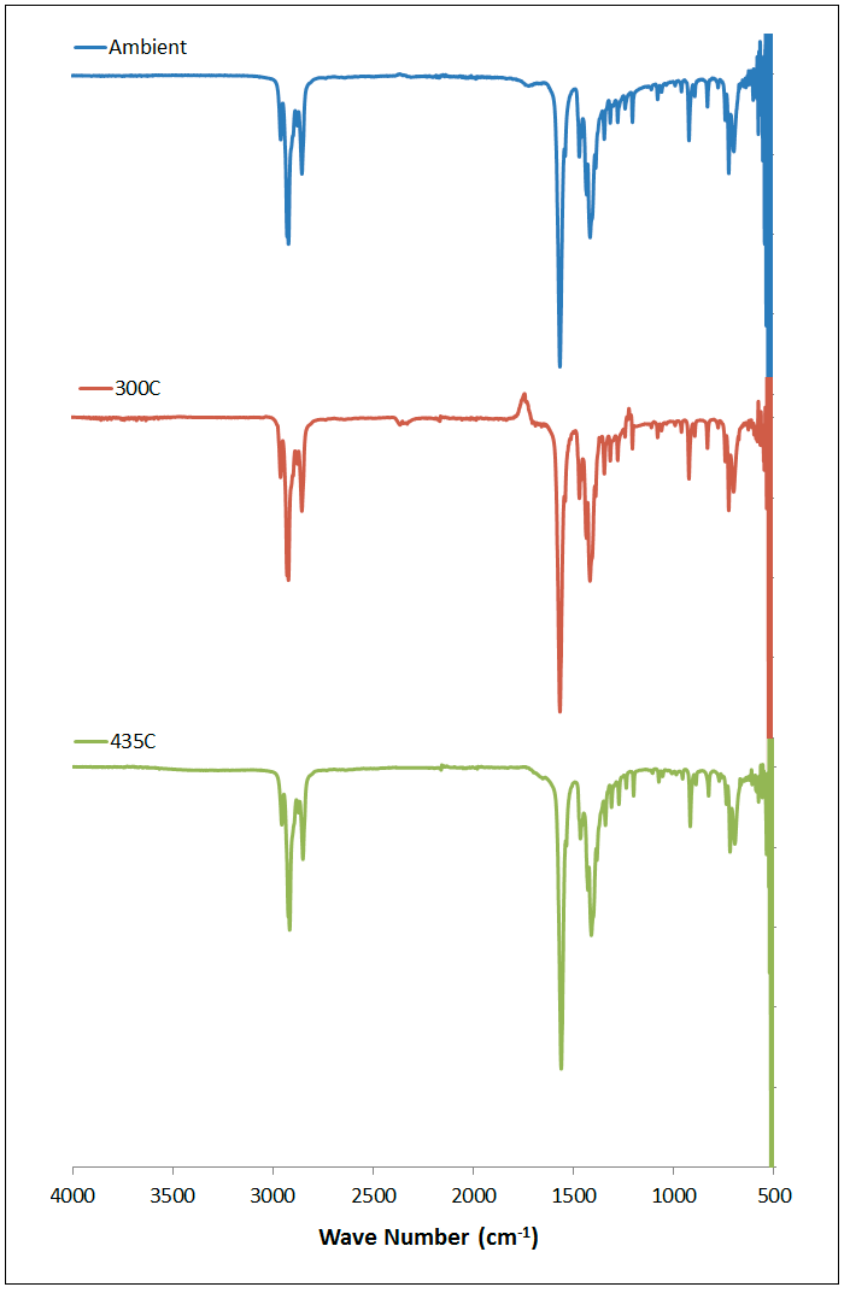


**Figure S23.** IR spectra of potassium decanoate collected over the wave number region $\tilde{\nu}/cm^{-1}$ = (4000 to 500) before melting, after melting to a liquid crystal phase and after clearing to an isotropic liquid phase.

*3.11. Potassium undecanoate*

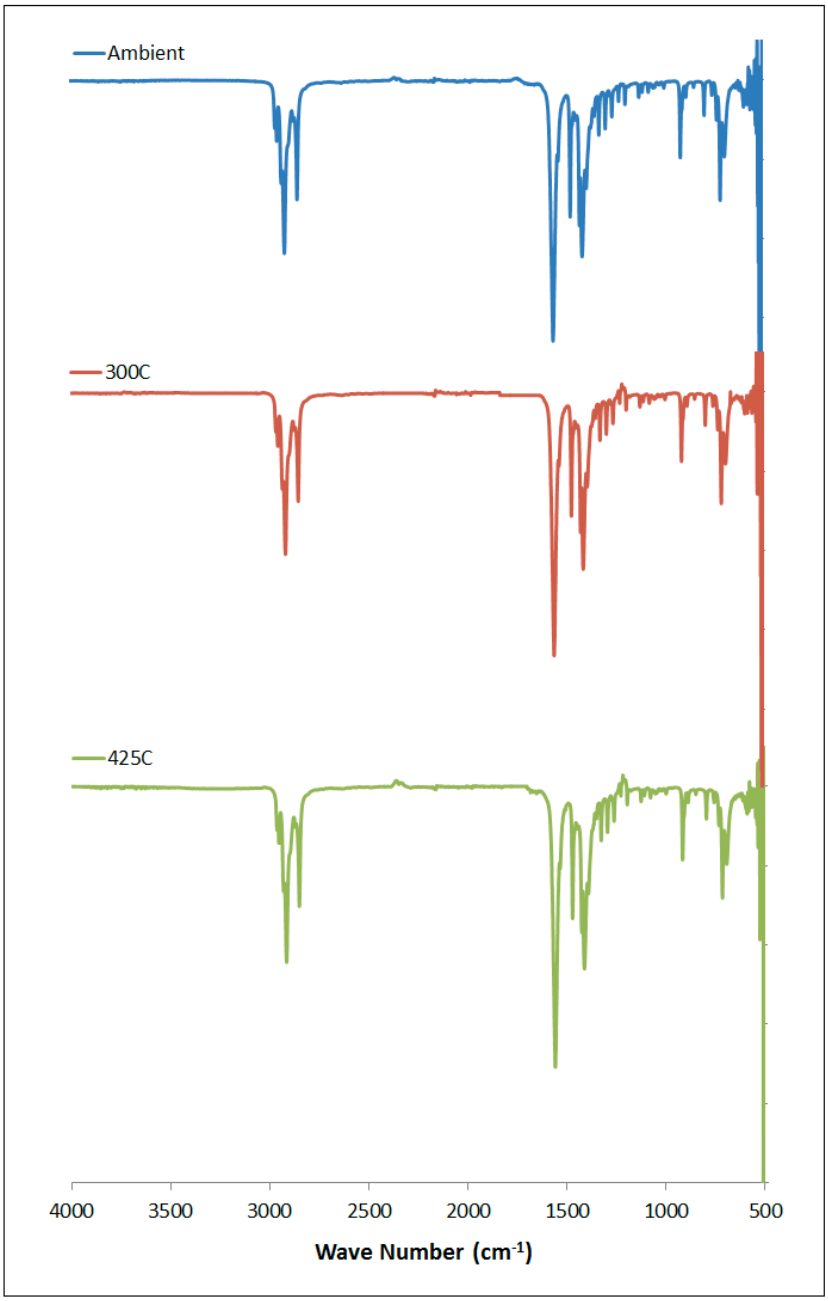


**Figure S24.** IR spectra of potassium undecanoate collected over the wave number region $\nu$/cm$^{-1}$ = (4000 to 500) before melting, after melting to a liquid crystal phase and after clearing to an isotropic liquid phase.

*3.12. Potassium dodecanoate (laurate)*

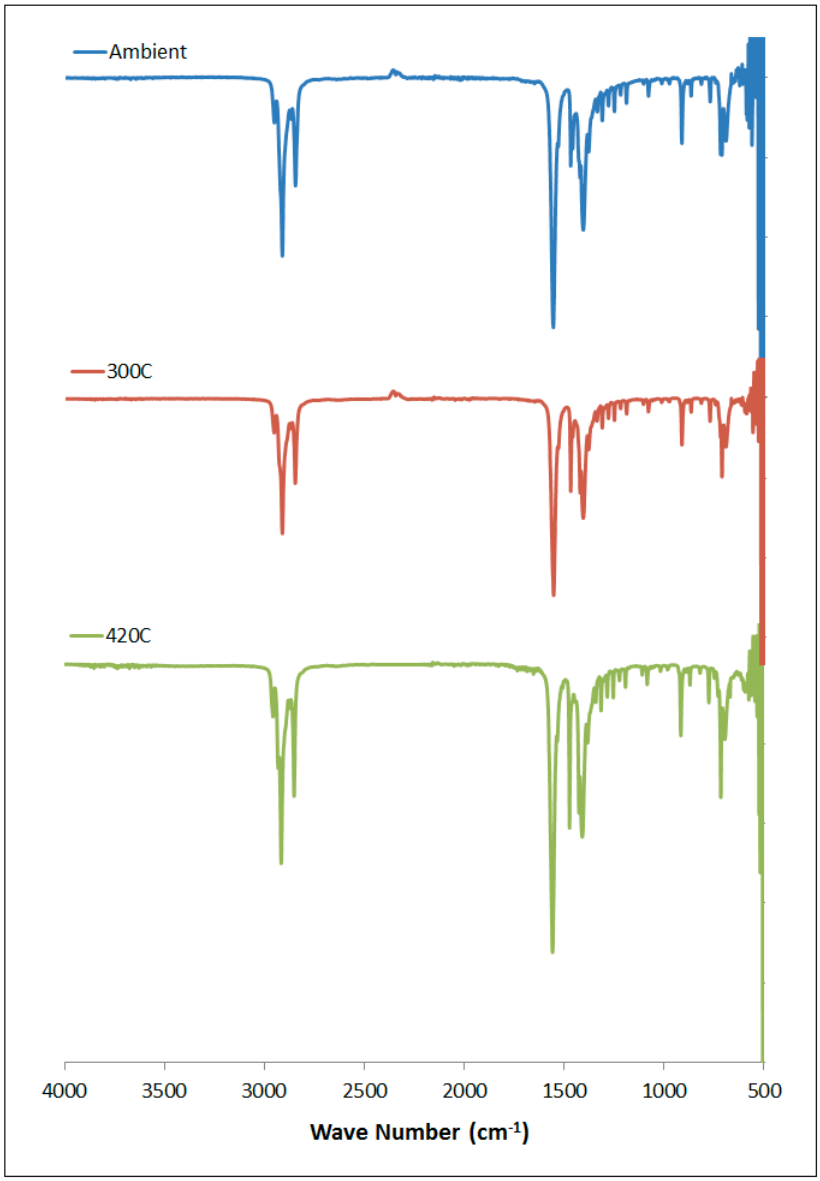


**Figure S25.** IR spectra of potassium dodecanoate collected over the wave number region $\nu/cm^{-1}$ = (4000 to 500) before melting, after melting to a liquid crystal phase and after clearing to an isotropic liquid phase.

## 4. Raman Spectra

### *4.1. Potassium methanoate (formate)*

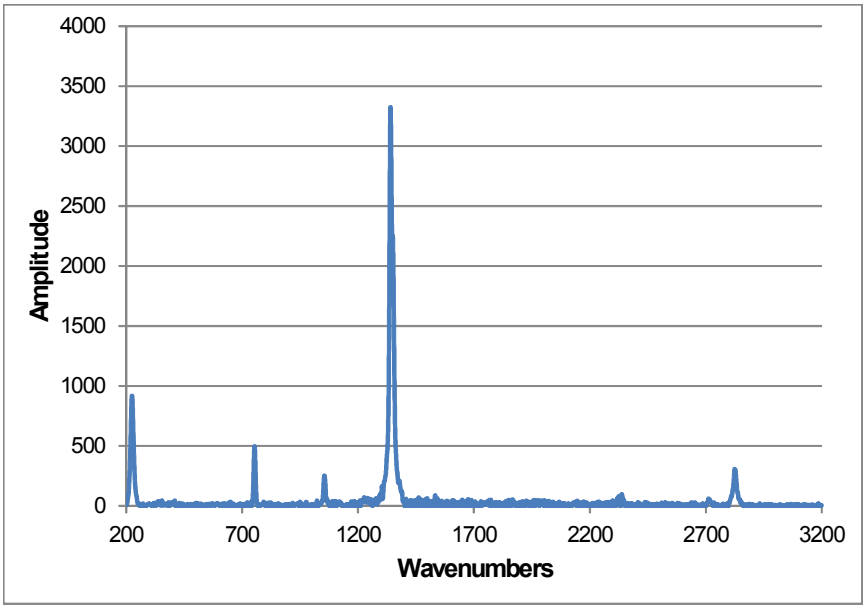


**Figure S26.** Raman spectrum of potassium methanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

### *4.2. Potassium Ethanoate (acetate)*

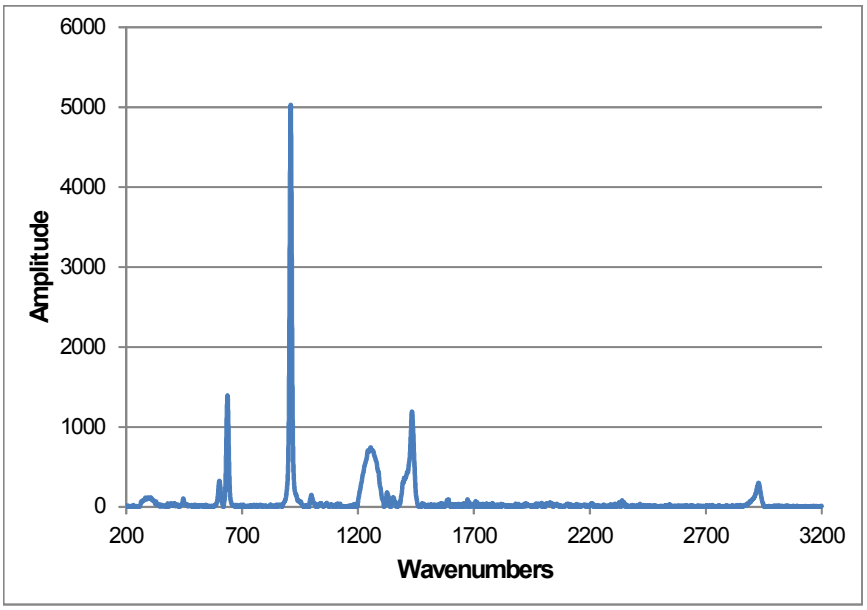


**Figure S27.** Raman spectrum of potassium ethanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.3. Potassium Propanoate*

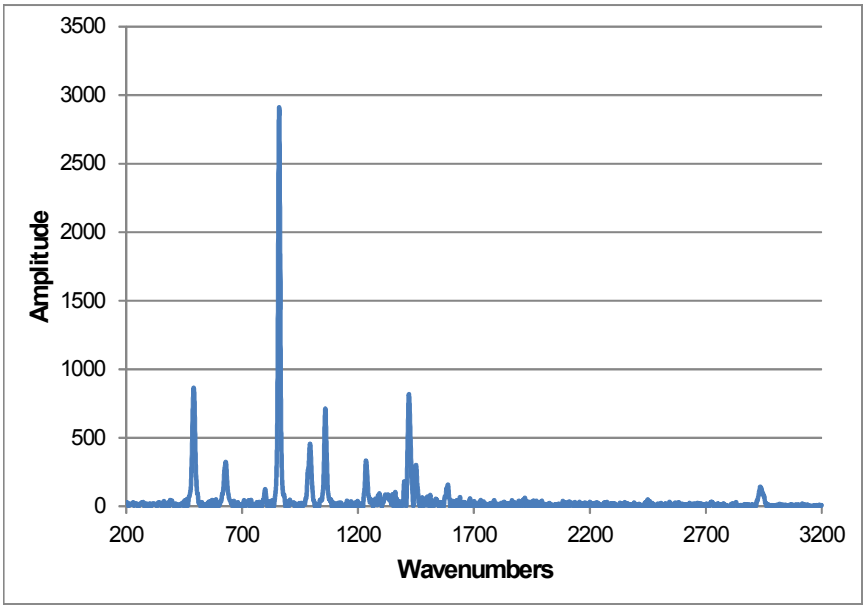


**Figure S28.** Raman spectrum of potassium propanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.4. Potassium Butanoate (butyrate)*

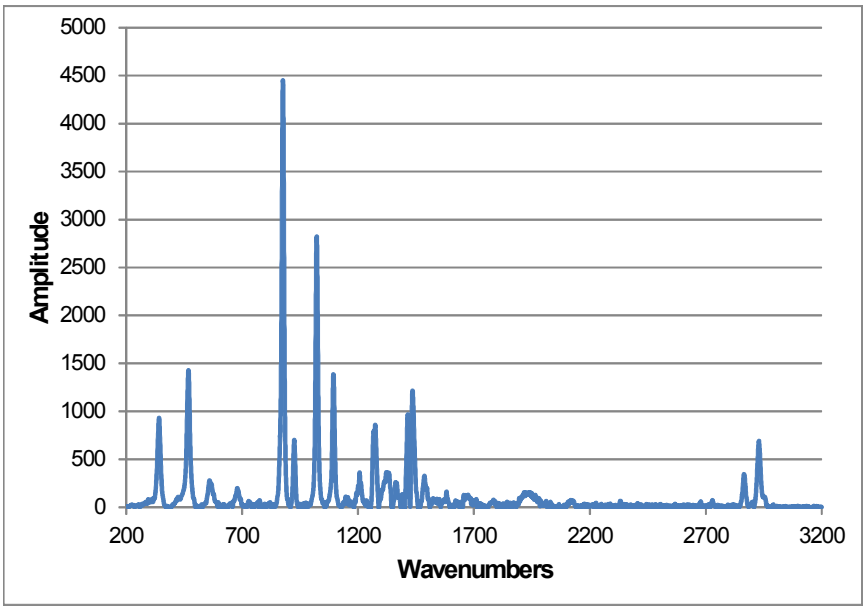


**Figure S29.** Raman spectrum of potassium butanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.5. Potassium Pentanoate (valerate)*

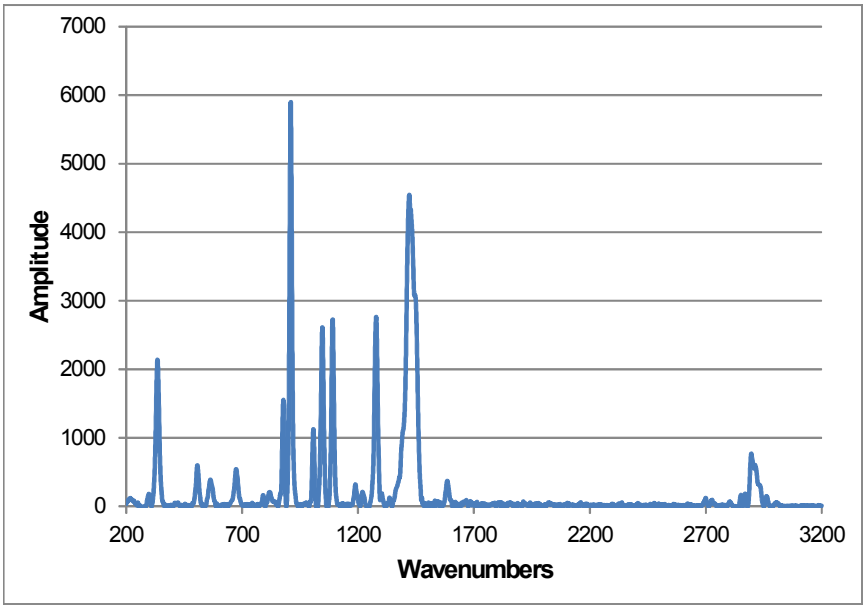


**Figure S30.** Raman spectrum of potassium pentanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.6. Potassium Hexanoate (caproate)*

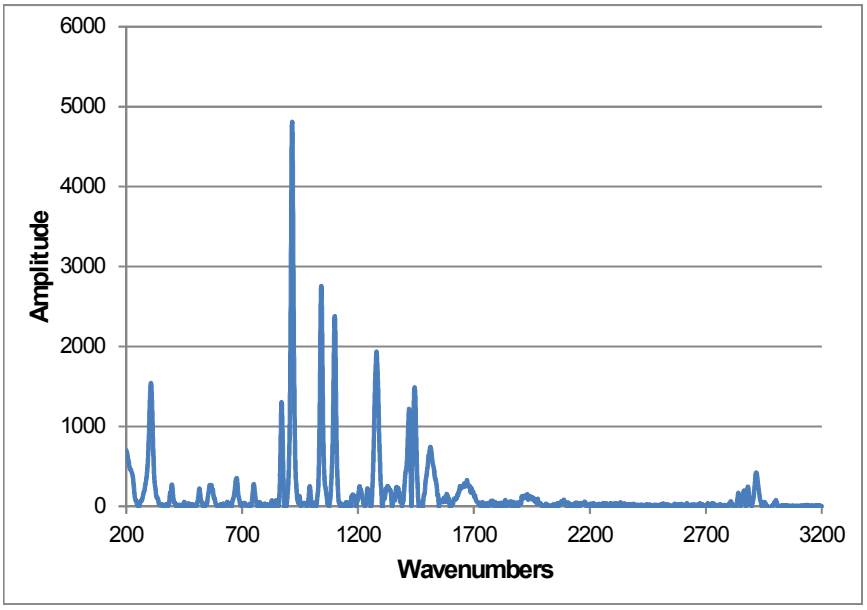


**Figure S31.** Raman spectrum of potassium hexanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.7. Potassium Heptanoate*

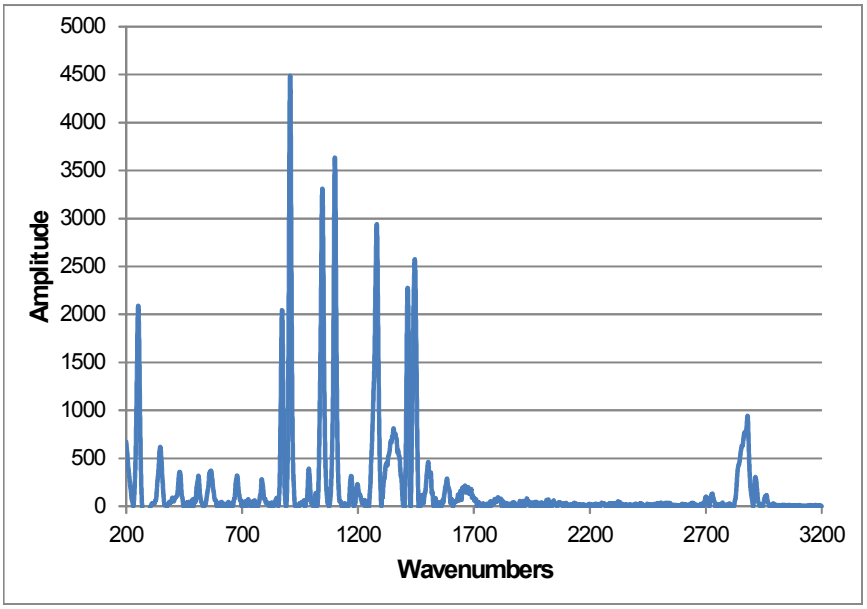


**Figure S32.** Raman spectrum of potassium heptanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.8. Potassium Octanoate (caprylate)*

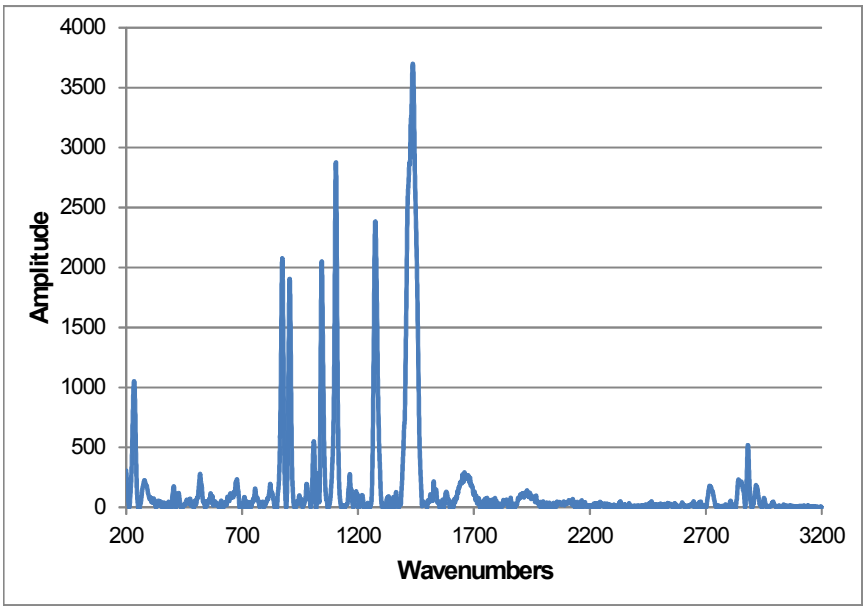


**Figure S33.** Raman spectrum of potassium octanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.9. Potassium Nonanoate (pelargonate)*

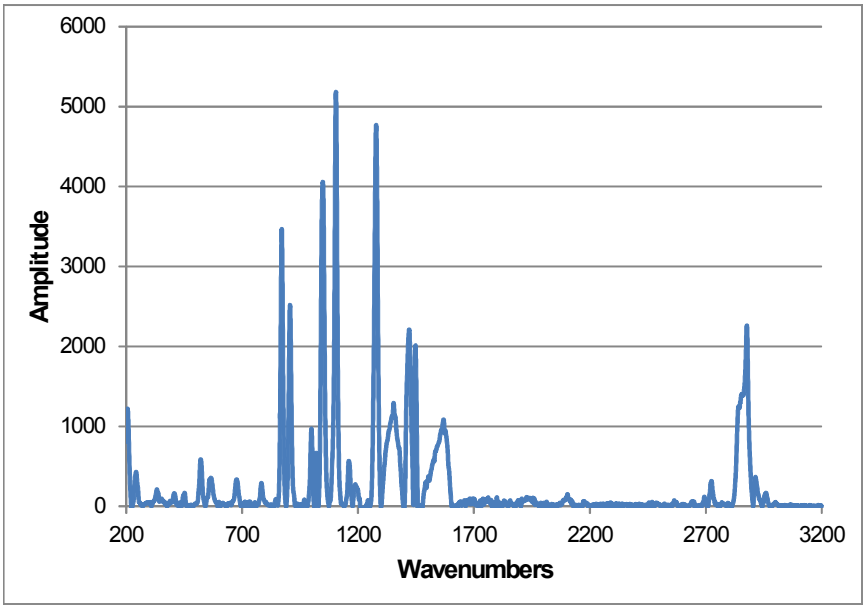


**Figure S34.** Raman spectrum of potassium nonanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.10. Potassium Decanoate (caprate)*

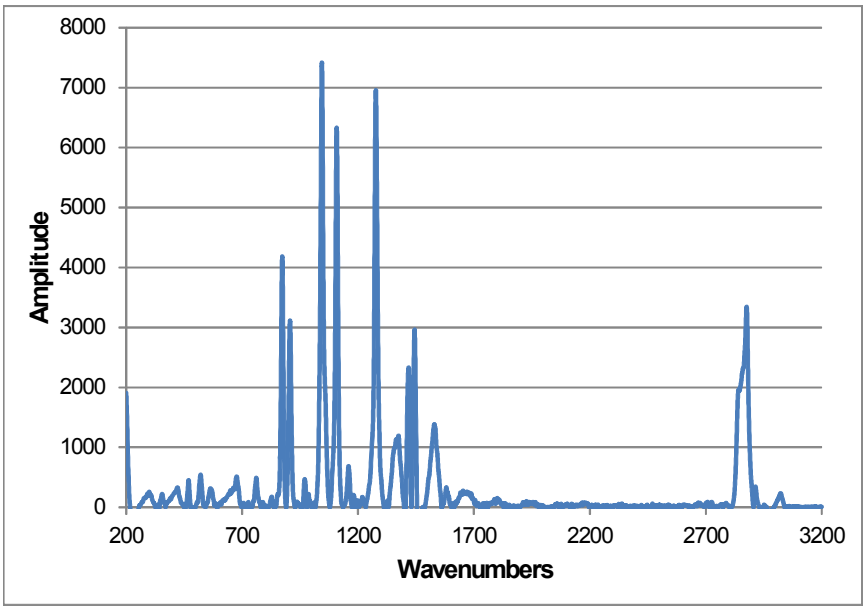


**Figure S35.** Raman spectrum of potassium decanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.11. Potassium Undecanoate*

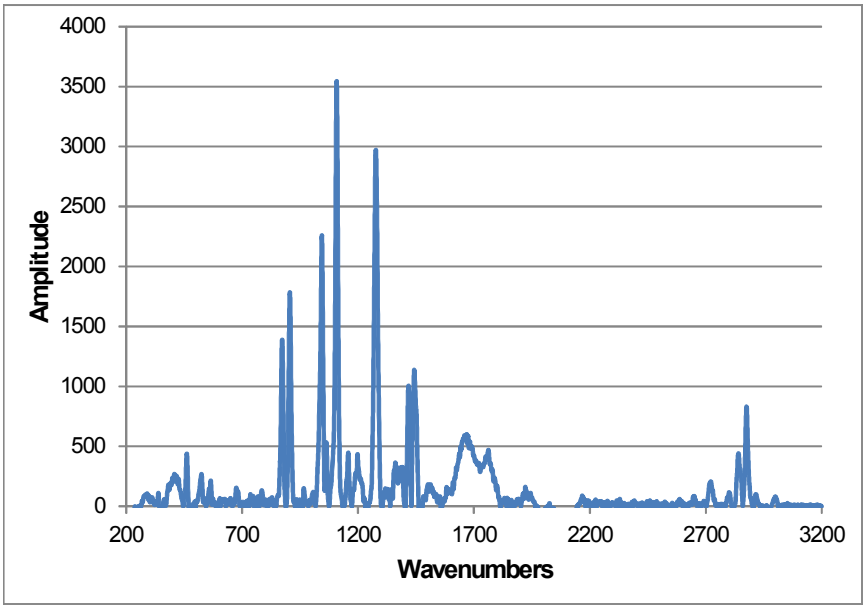


**Figure S36.** Raman spectrum of potassium undecanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

*4.12. Potassium Dodecanoate (laurate)*

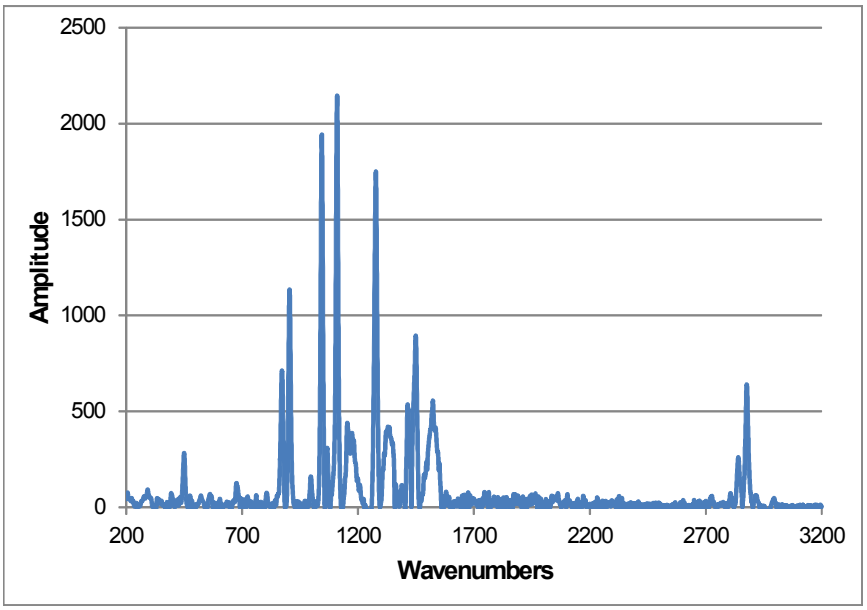


**Figure S37.** Raman spectrum of potassium dodecanoate over the wave number region $\nu/cm^{-1}$ = (3200 to 200).

## 5. Ultraviolet-visible spectrometry

### *5.1. Potassium Methanoate*

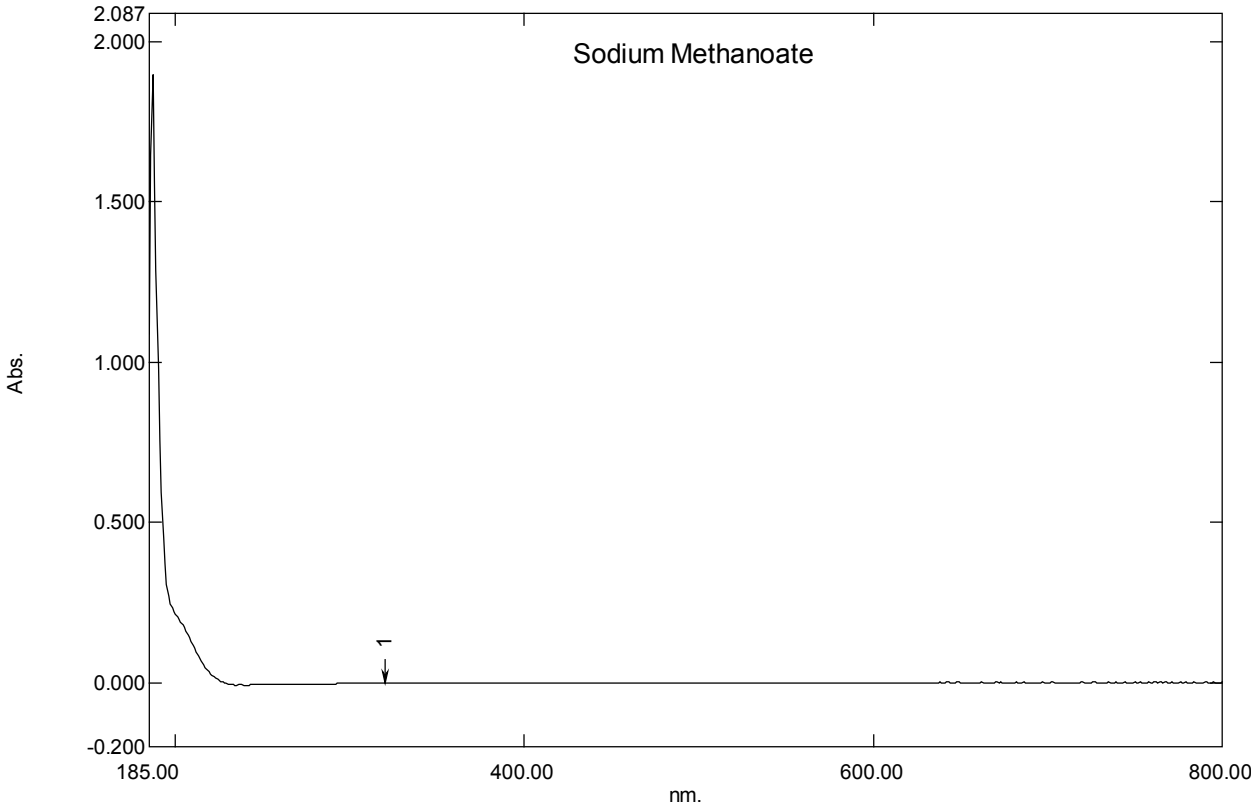


**Figure S38.** UV–vis spectrum of potassium methanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.2. Potassium Ethanoate*

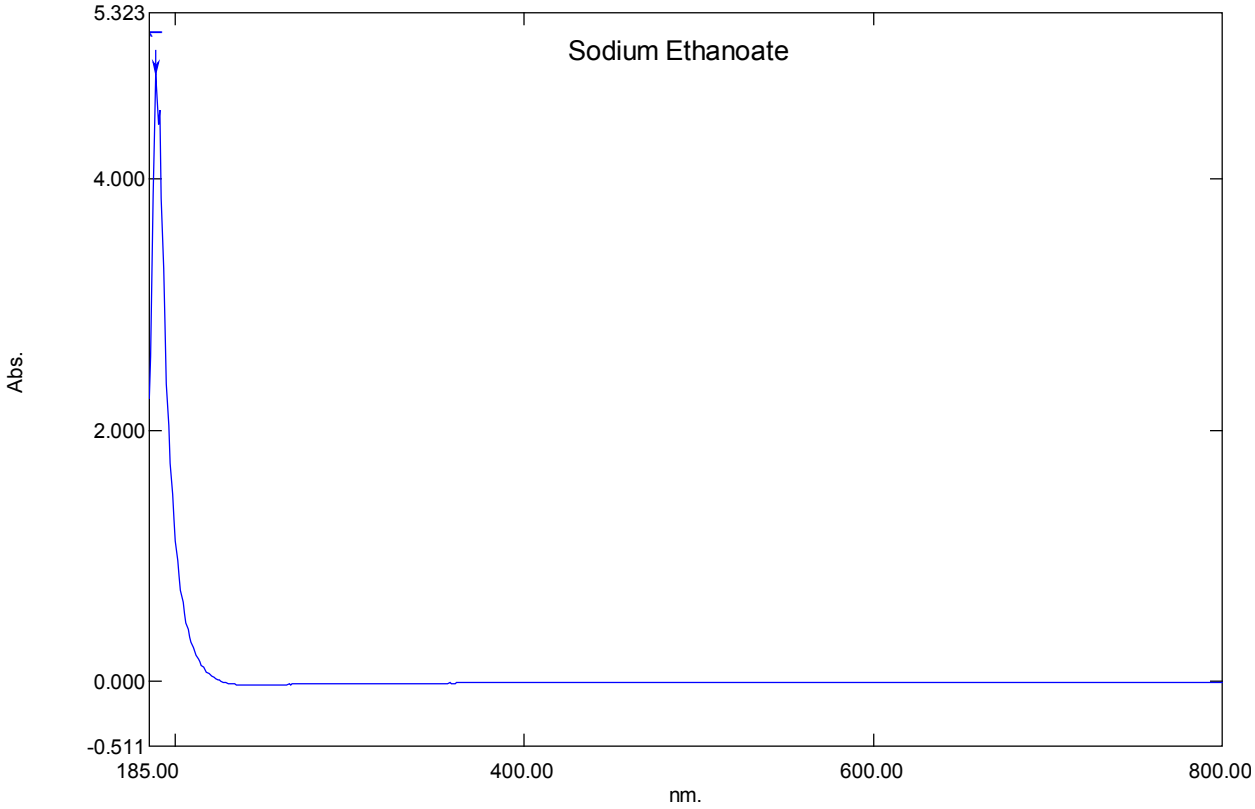


**Figure S39.** UV–vis spectrum of potassium ethanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.3. Potassium Propanoate*

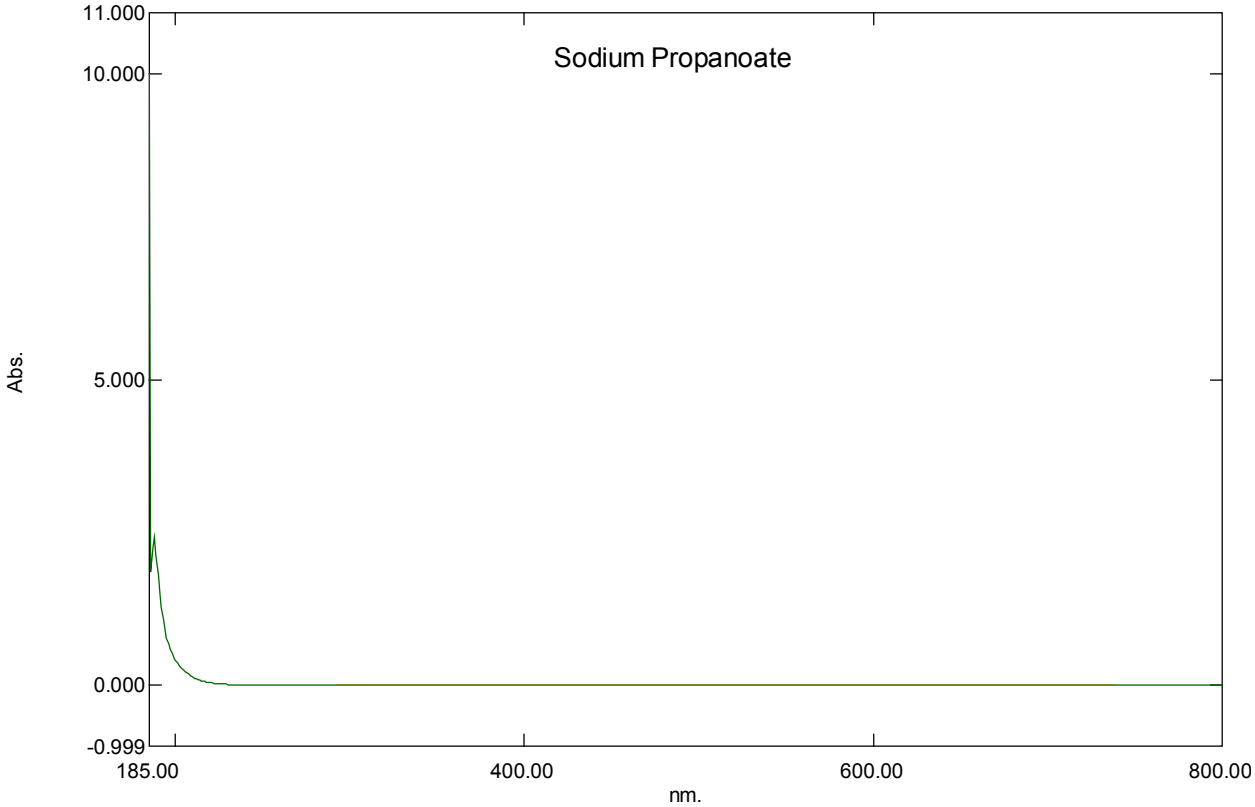


**Figure S40.** UV–vis spectrum of potassium propanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.4. Potassium Butanoate (butyrate)*

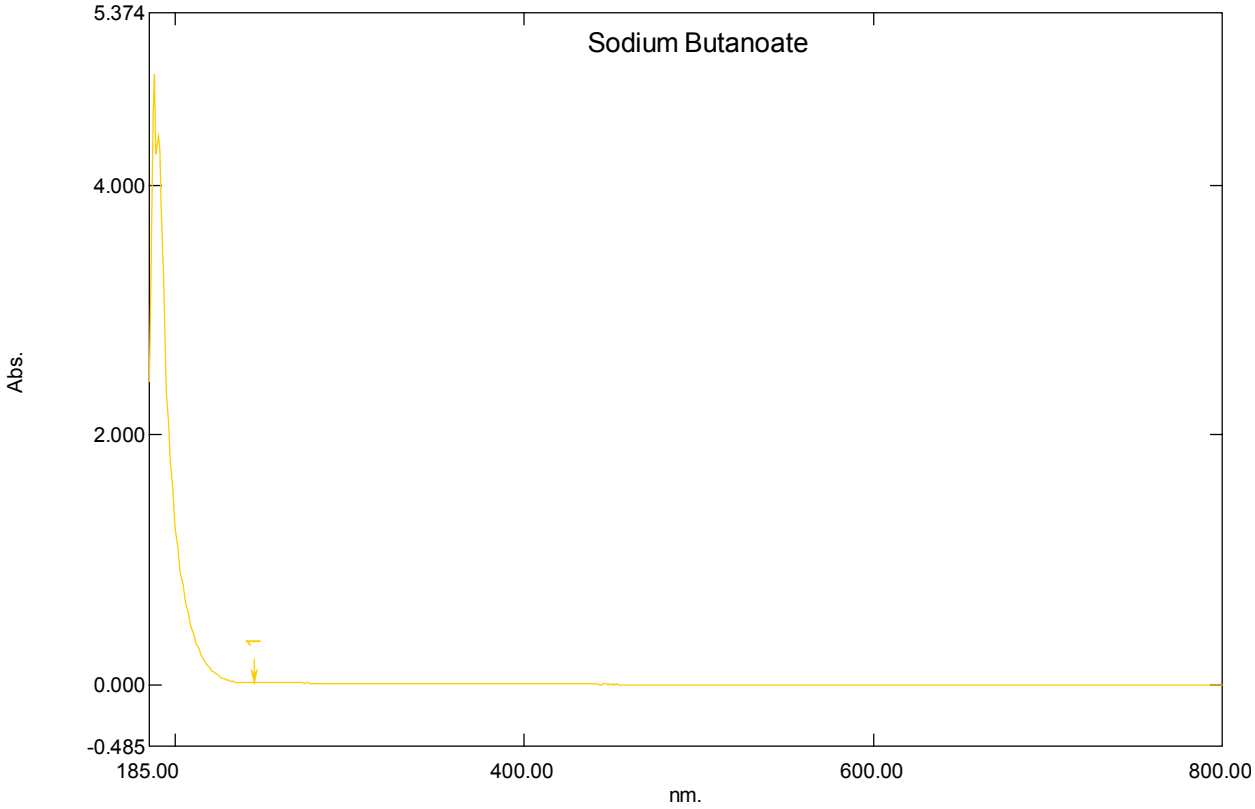


**Figure S41.** UV–vis spectrum of potassium butanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.5. Potassium Pentanoate (valerate)*

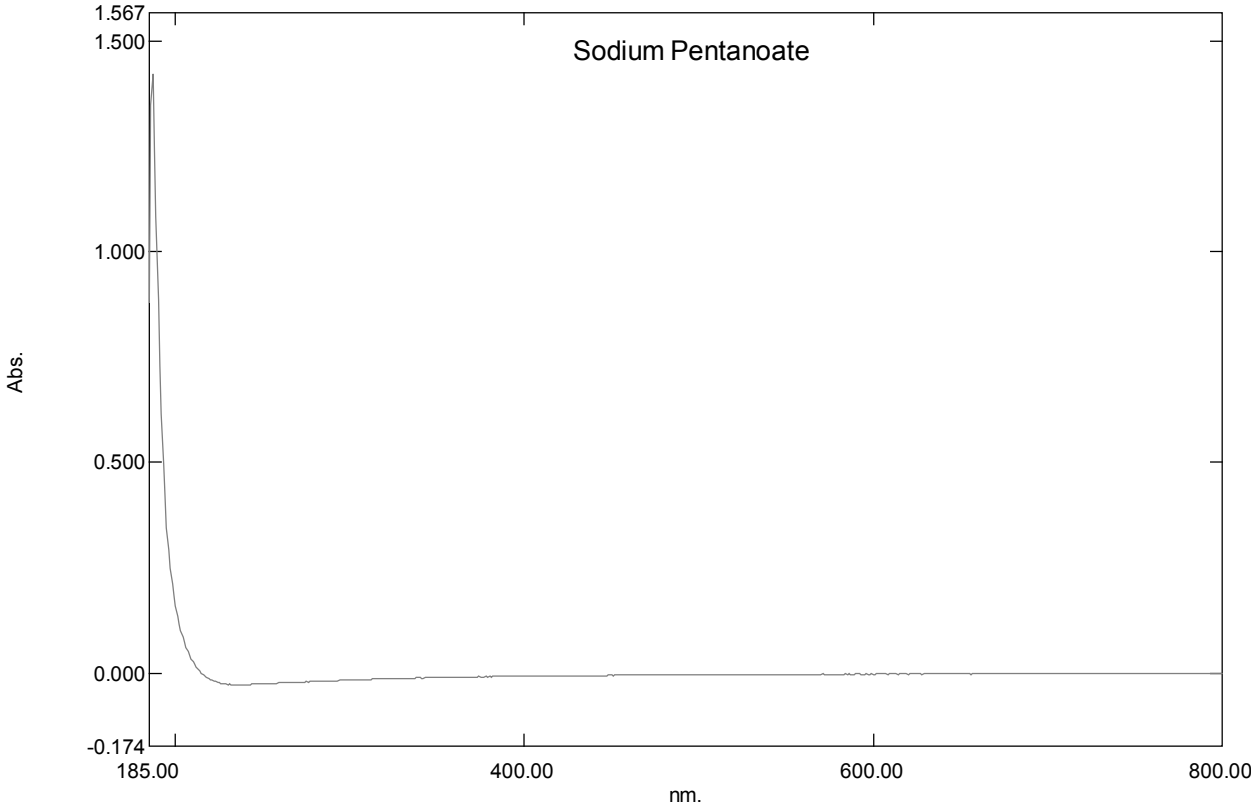


**Figure S42.** UV–vis spectrum of potassium pentanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.6. Potassium Hexanoate (caproate)*

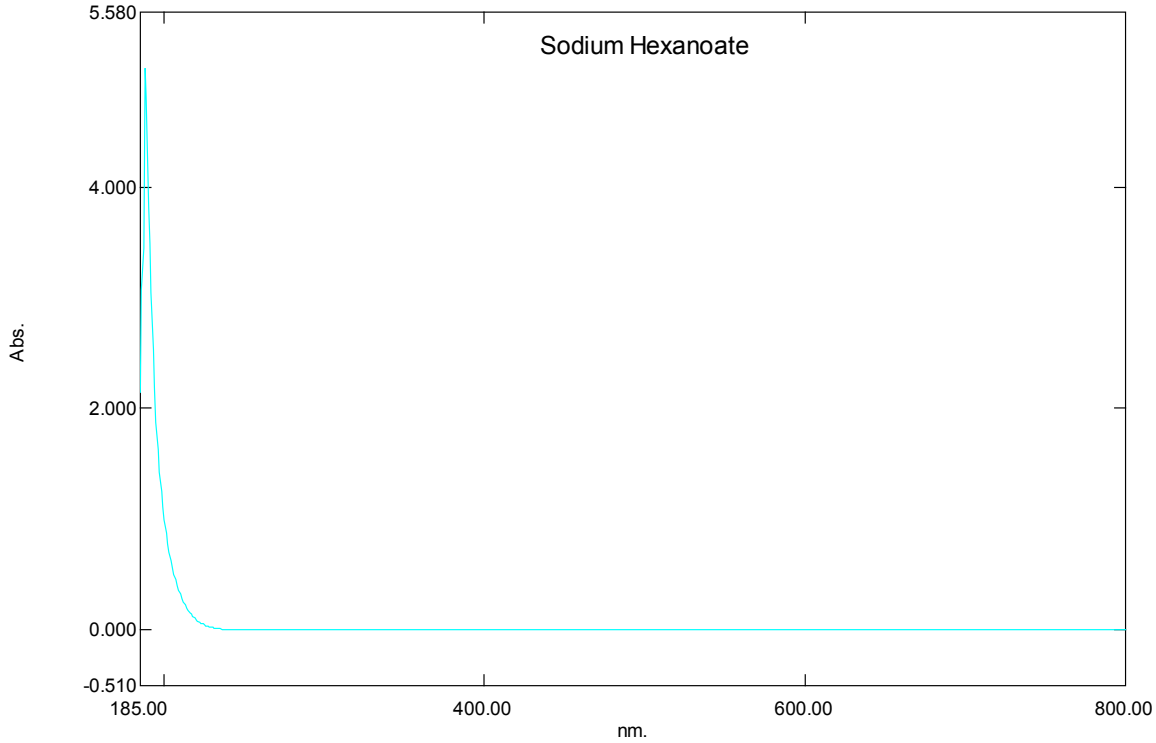


**Figure S43.** UV–vis spectrum of potassium hexanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.7. Potassium Heptanoate*

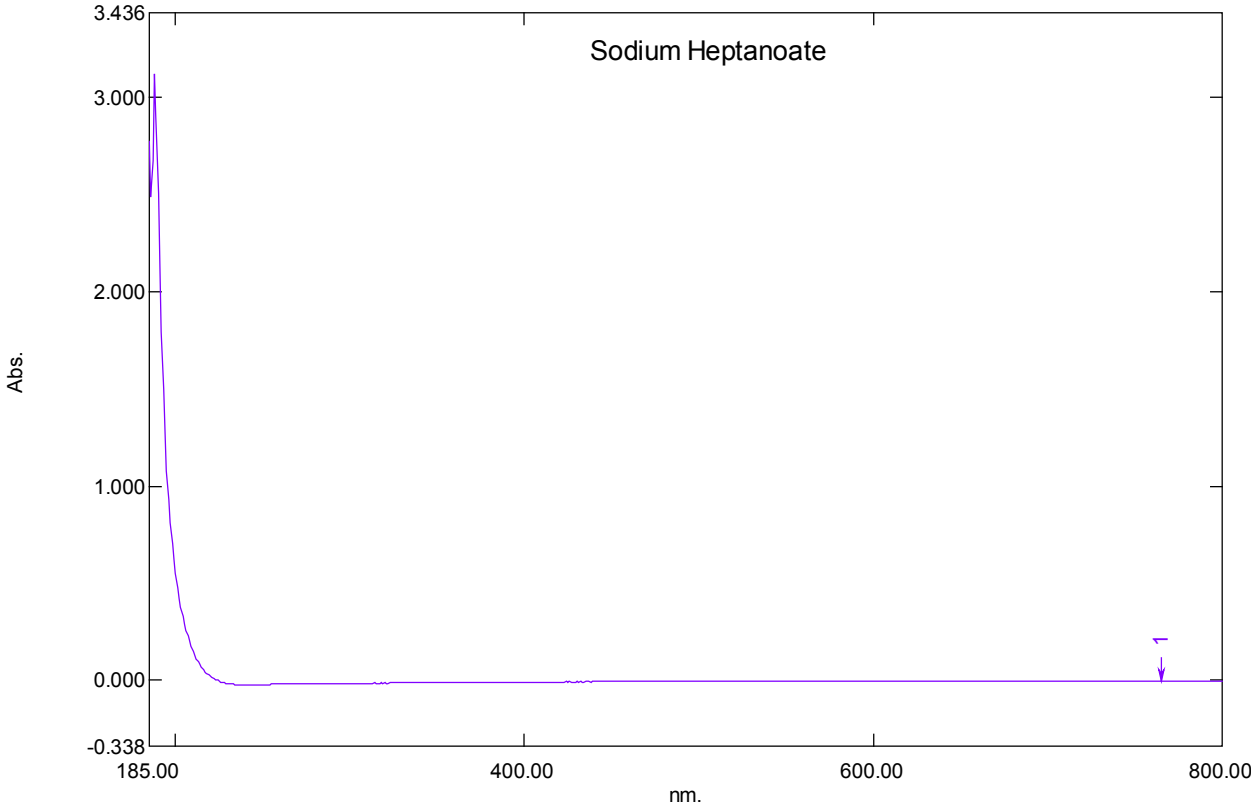


**Figure S44.** UV–vis spectrum of potassium heptanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.8. Potassium Octanoate (caprylate)*

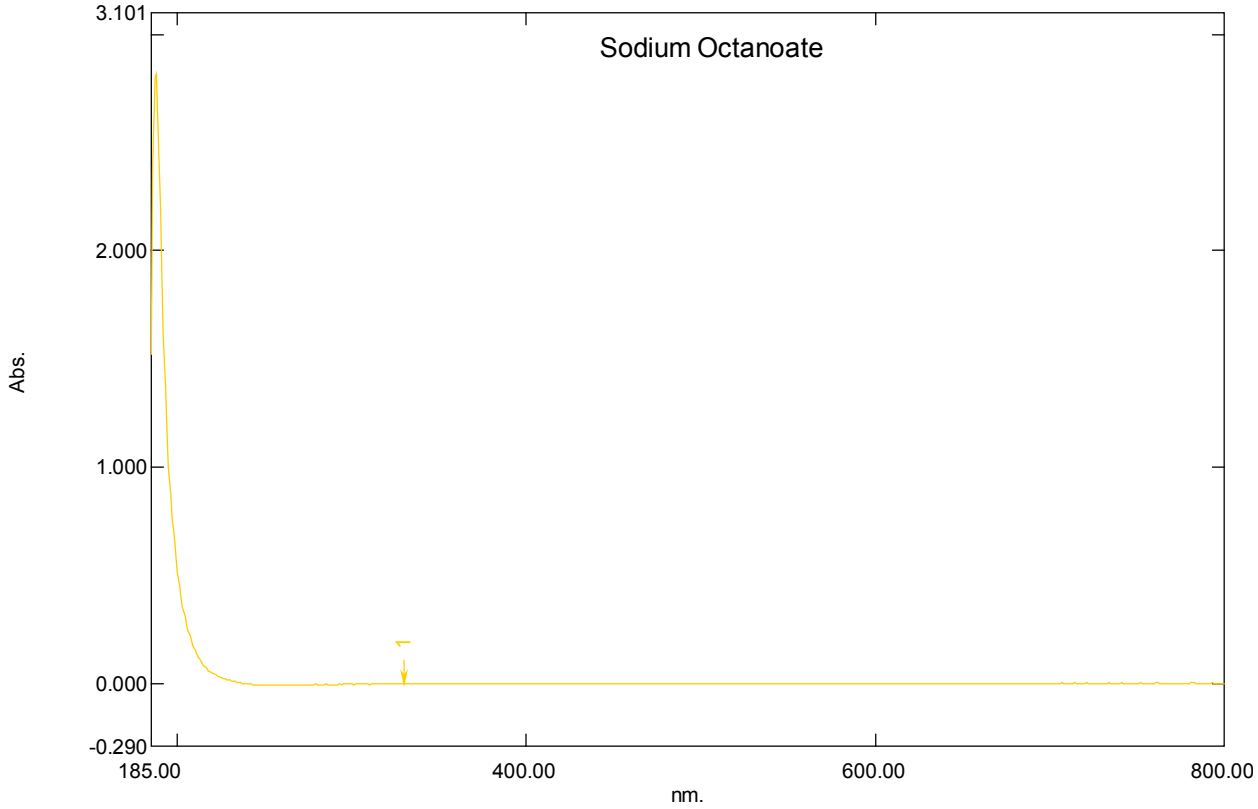


**Figure S45.** UV–vis spectrum of potassium octanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.9. Potassium Nonanoate (pelargonate)*

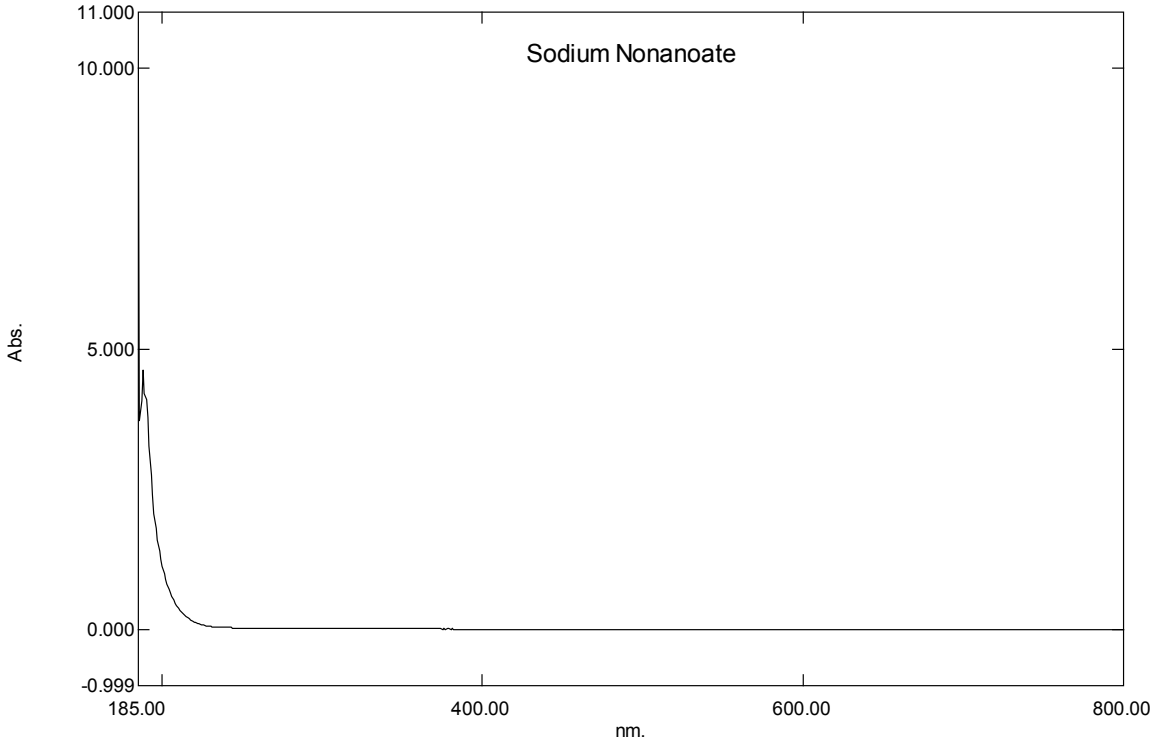


**Figure S46.** UV–vis spectrum of potassium nonanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.10. Potassium Decanoate (caprate)*

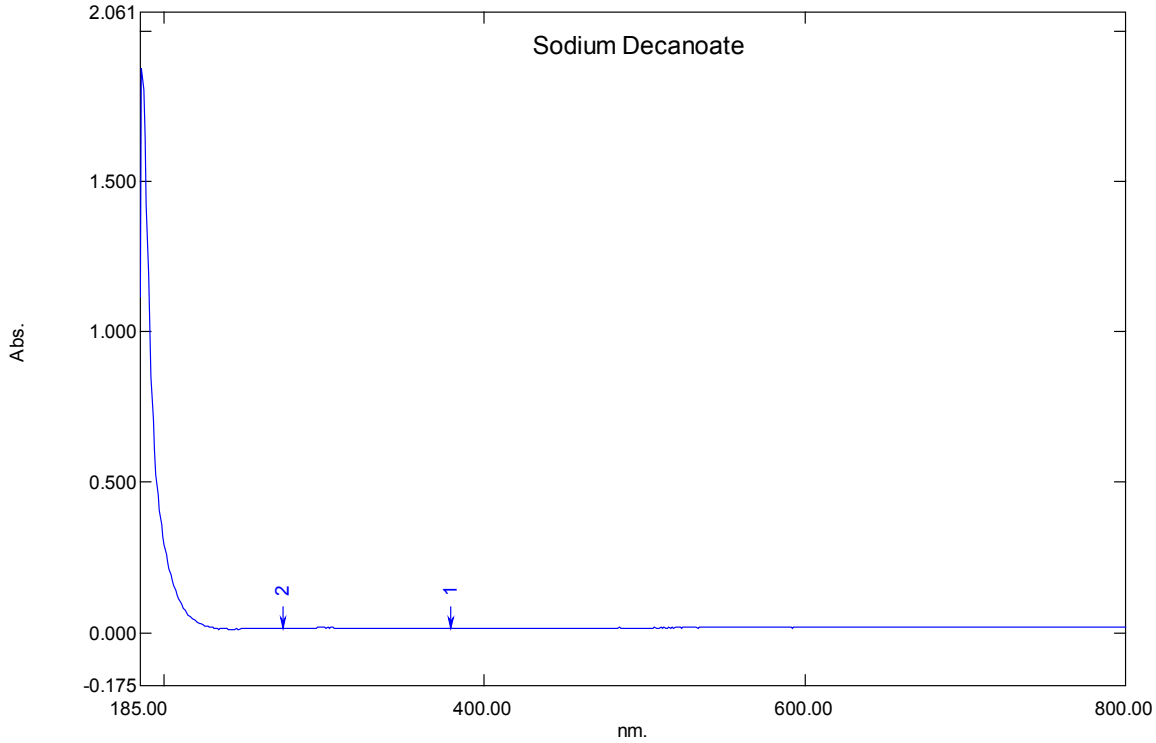


**Figure S47.** UV–vis spectrum of potassium decanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.11. Potassium Undecanoate*

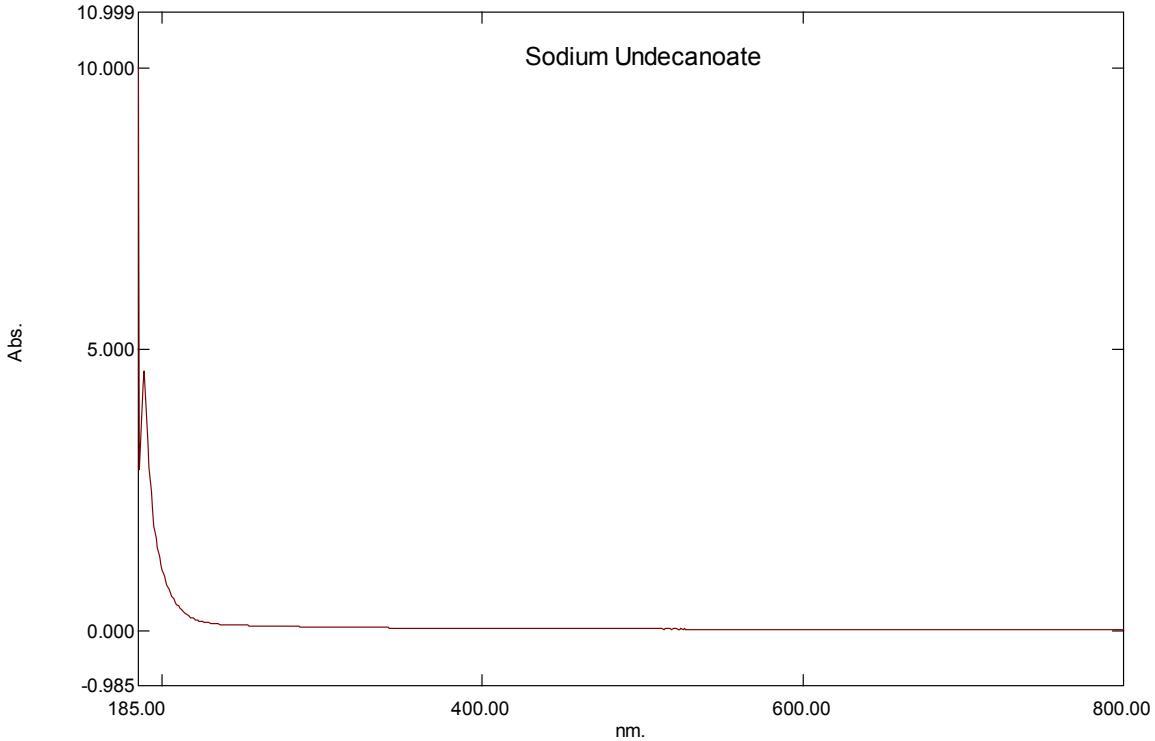


**Figure S48.** UV–vis spectrum of potassium undecanoate in the wavelength range $\lambda$/nm = (185 to 800).

*5.12. Potassium Dodecanoate (laurate)*

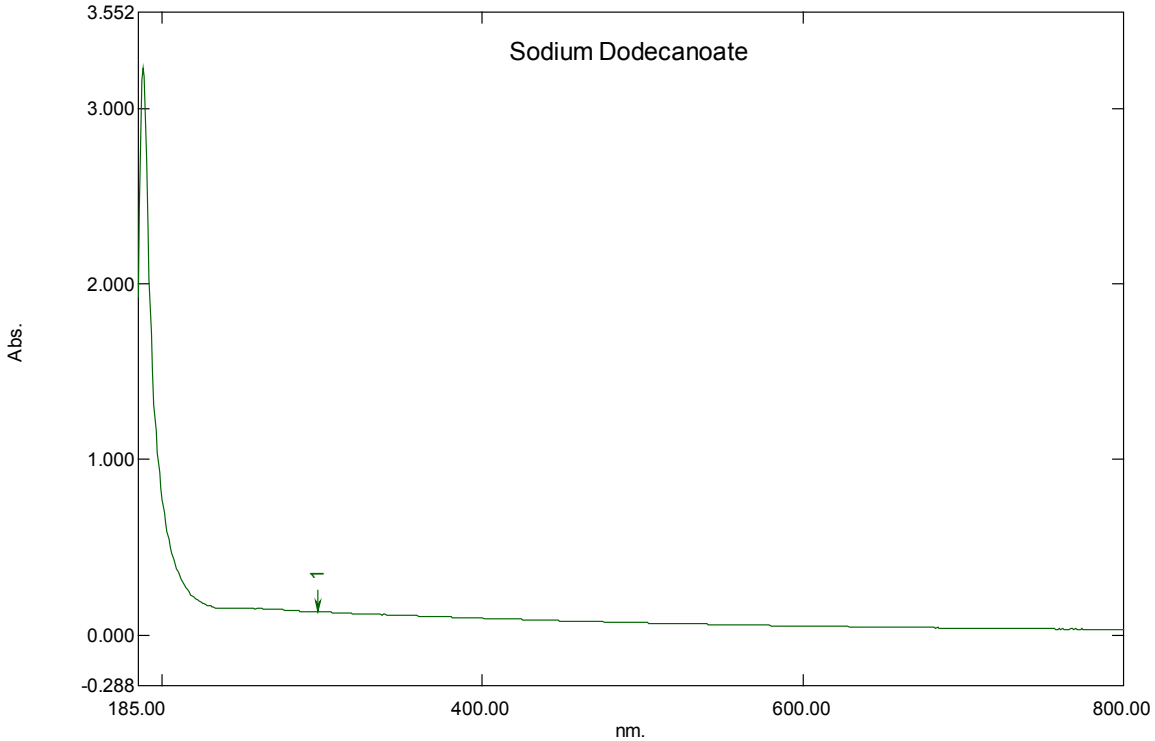


**Figure S49.** UV–vis spectrum of potassium dodecanoate in the wavelength range $\lambda$/nm = (185 to 800).