# Preparation of Pear Essence (Propyl Acetate) (7A/PPE)

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07/11/2017

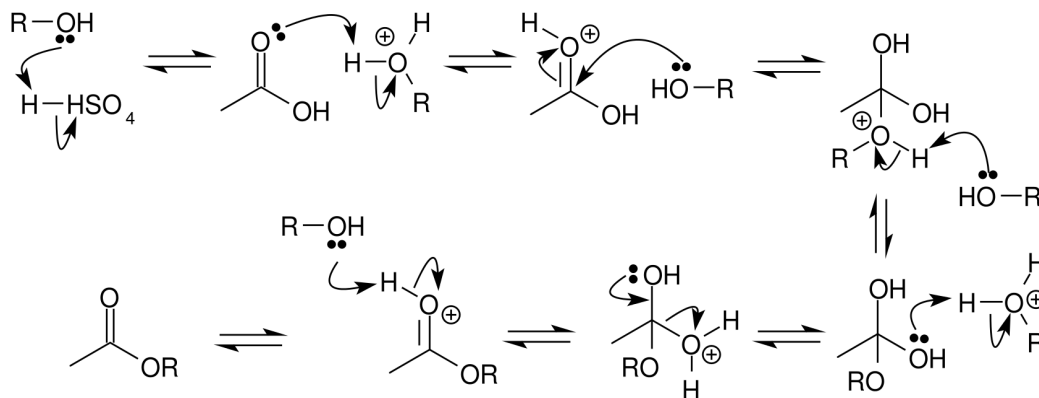## 1 Reaction Mechanism[1] and Overall Equation



Figure 1: Mechanism for reaction
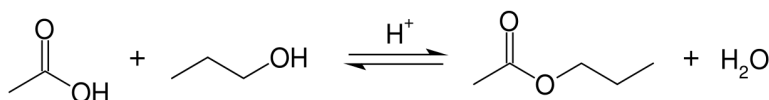


Figure 2: Overall Equation for Reaction

## 2 Results and Analysis

Boiling temperature of pure product: $101\,°C$

Mass of pure product: $4.43\,g$

### 2.1 Yield Calculation

$$\text{Moles of propan-1-ol at start of reaction} = \frac{9.6\,g}{(3(12.011) + 8(1.008) + 15.999)\ g\,mol^{-1}}$$

$$= \frac{9.6\,g}{60.096\,g\,mol^{-1}} = 0.16\,mol$$

$$\text{Moles of acetic acid at start of reaction} = \frac{24\,g}{(2(12.011) + 4(1.008) + 2(15.999))\ g\,mol^{-1}}$$

$$= \frac{24\,g}{60.052\,g\,mol^{-1}} = 0.40\,mol$$

From the equation shown in figure 2 there is a 1:1 molar ratio between propan-1-ol and acetic acid, hence the acetic acid is in excess. The equation also shows a 1:1 molar ratio between the propan-1-ol and propyl acetate, hence the theoretical amount of propyl acetate produced is $0.16\,mol$.

$$\therefore \text{Theoretical yield of propyl acetate} = 0.16\,mol \times (5(12.011) + 10(1.008) + 2(15.999))\ g\,mol^{-1}$$

$$= 0.16\,mol \times 102.133\,g\,mol^{-1} = 16\,g$$

$$\therefore \text{Percentage yield} = \frac{4.43\,g}{16\,g} \times 100\,\% = 27\,\%$$

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[1] David Klein. *Organic Chemistry.* 2nd ed. Wiley, 2015, Preparation of Esters, p. 1014.

This is quite low. This may be due to losses during the purification (e.g. containers were not washed after transfers and some product remained in the filter paper) and a consequence of the reversible nature of the reaction.

## 2.2 Spectra

Table 1: IR Spectrum of propan-1-ol.

| Wavenumber / cm$^{-1}$ | Strength | Assignment |
|---|---|---|
| 2976.7 | Weak | $CH_3$ Absorption |
| 2936.0 | Weak | $C-H_2$ Absorption |
| 2962.3 | Weak | $C-H_3$ Absorption |
| 3319.0 | Weak and Broad | $O-H$ Absorption in Alcohol |

Table 2: $^1$H NMR Spectrum of propan-1-ol.

| Chemical Shift / ppm | $J$-Coupling | Integral Area | Summary |
|---|---|---|---|
| Approx. 7.3 | Singlet | Not Integrated | Characteristic for CDCl$_3$ (Solvent) |
| 3.66 | Triplet | 0.99 | Two $\alpha$-protons to alcohol group. Coupled to two protons. |
| 2.03 | Singlet | 3.00 | OH proton. Exchange decoupled. |
| 1.57 | Quintet (Unclear) | (Integrated together) | Additional splitting possibly obscured by adjacent peaks. Coupled to four or five protons. |
| 1.00 | Triplet (Small right-hand peak) | | Coupled to two protons. |

Table 3: IR Spectrum of acetic acid.

| Wavenumber / cm$^{-1}$ | Strength | Assignment |
|---|---|---|
| 1703.9 | Strong | C=O Absorption close to acid range (1725-1705 cm$^{-1}$) |
| 3032.6 | Weak and Broad | $O-H$ Absorption close to carboxylic acid range (3000-2500 cm$^{-1}$) |

Table 4: $^1$H NMR Spectrum of acetic acid.

| Chemical Shift / ppm | $J$-Coupling | Integral Area | Summary |
|---|---|---|---|
| 10.67 | Singlet | 0.90 | Single proton in $-$COOH group. Exchange decoupled. |
| Approx. 7.4 | Singlet | Not Integrated | Characteristic for CDCl$_3$ (Solvent). |
| 2.19 | Singlet | 3.00 | Three $\alpha$-protons to carboxyl group. |

Table 5: IR Spectrum of Product.

| Wavenumber / cm$^{-1}$ | Strength | Assignment |
|---|---|---|
| 1738.0 | Strong | C=O Absorption in the ester range (1740-1710 cm$^{-1}$) |
| 2882.5 | Weak | $C-H$ Absorption |
| 2970.5 | Weak | $C-H$ Absorption |

Table 6: $^1$H NMR Spectrum of Product.

| Chemical Shift / ppm | $J$-Coupling | Integral Area | Summary |
|---|---|---|---|
| Approx. 7.4 | Singlet | 0.030 | Characteristic for CDCl$_3$ (Solvent) |
| 4.14 | Triplet | 1.98 | Two protons (RCOO$-$C$\underline{H}$). Coupled to two protons. |
| 2.17 | Singlet | 3.28 | Three protons in unique environment |
| Approx. 1.8 | Quartet (Unclear) | 1.90 | Two protons coupled three or four protons: splitting pattern difficult to interpret. |
| 1.06 | Triplet (Small right-hand peak) | 2.75 | Three protons coupled to two protons. |

These spectra are consistent with propyl acetate as a product since the starting materials both had a broad peak corresponding to $O-H$ absorptions in their IR spectra, however this is absent in the product's IR spectrum. Also the NMR spectrum for the product shows it has four distinct hydrogen environments with the expected chemical shifts and (mostly) the expected splitting pattens for propyl acetate. In the IR spectra the C=O absorption has shifted position from being at 1703.9 cm$^{-1}$ in acetic acid to 1738.0 cm$^{-1}$ in the product: this higher wavenumber is expected for the production of an ester.