

Supplementary Information

Investigation of factors affecting isolation of needle-shaped particles in a vacuum agitated filter drier through non-invasive measurements by Raman spectrometry

Peter Hamilton,^a David Littlejohn,^{a*} Alison Nordon,^{a*} Jan Sefcik,^b Paul Slavin,^c John Andrews^d and Paul Dallin^d

^a WestCHEM, Department of Pure and Applied Chemistry and CPACT, University of Strathclyde, Glasgow, G1 1XL, UK

^b Department of Chemical and Process Engineering, University of Strathclyde, 75 Montrose Street, Glasgow, G1 1XJ, UK

^c GlaxoSmithKline, Gunnels Wood Road, Stevenage, Hertfordshire, SG1 2NY, UK

^d Clairet Scientific, 17/18 Scirocco Close, Moulton Park Industrial Estate, Northampton, NN3 6AP, UK

* denotes authors to whom correspondence should be sent

David Littlejohn

Email: d.littlejohn@strath.ac.uk; tel: +44(0)141 548 2067; fax: +44(0)141 548 4212

Alison Nordon

Email: alison.nordon@strath.ac.uk; tel: +44(0)141 548 3044; fax: +44(0)141 548 4212

Assignment of Raman spectra of cellobiose octaacetate (COA) and methanol

Underivatised and 1st derivative Raman spectra of COA and methanol are shown in Fig. S1a and Fig. S1b, respectively.

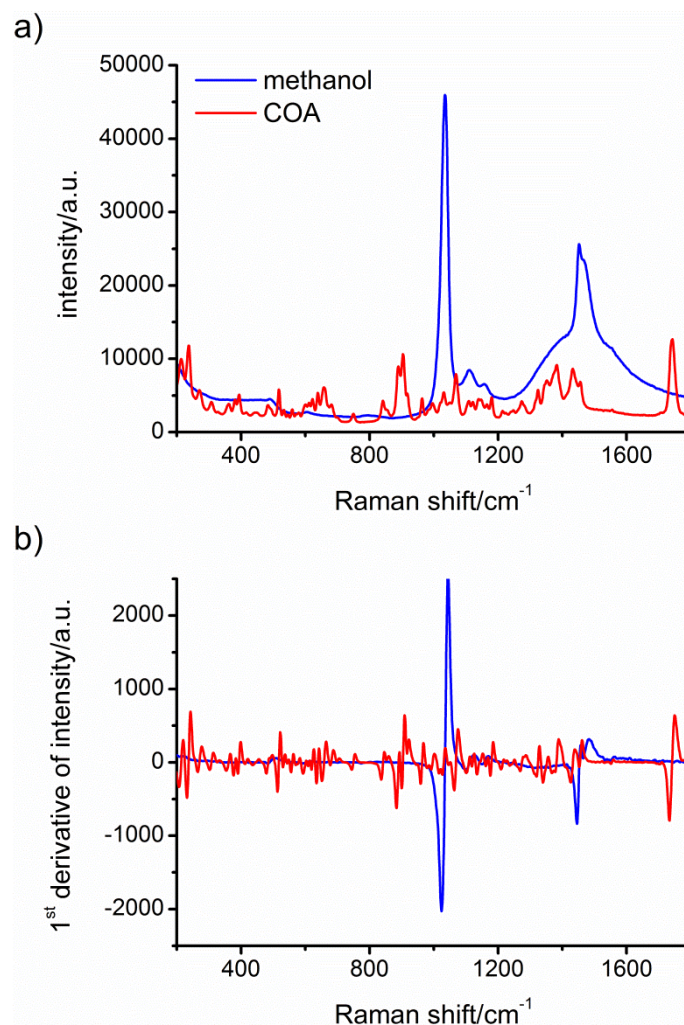


Fig. S1. a) Underivatised and b) 1st derivative Raman spectra of COA (red) and methanol (blue).

The methanol peaks at 1036 and 1453 cm⁻¹ in Fig. S1a can be attributed to the C-O stretch and CH₃ bending mode (Mammone et al., 1980). As the samples were contained within glass

vials and analysed from above, there is a broad peak at approximately 1500 cm^{-1} , which arises from the base of the glass vial, evident in the spectrum of methanol. The COA peaks in Fig. S1a can be assigned as follows (VanderHart et al., 1996): i) $900 - 1120\text{ cm}^{-1}$ arise from HCC and HCO bending at C6 and heavy-atom (C-C and C-O) stretching; ii) $1150 - 1330\text{ cm}^{-1}$ arise from heavy-atom (C-C and C-O) stretching and HCC and HCO bending; iii) $1350 - 1410\text{ cm}^{-1}$ arise from HCC, HCO and HOC bending; iv) $1420 - 1490\text{ cm}^{-1}$ arise from HCH and HOC bending; and v) the peak at 1743 cm^{-1} arises from the carbonyls in the acetyl groups.

References

- Mammone, J.F., Sharma, S.K., Nicol, M., 1980. Raman-spectra of methanol and ethanol at pressures up to 100 kbar. *Journal of Physical Chemistry* 84, 3130-3134.
- VanderHart, D.L., Hyatt, J.A., Atalla, R.H., Tirumalai, V.C., 1996. Solid-state C-13 NMR and Raman studies of cellulose triacetate: Oligomers, polymorphism, and inferences about chain polarity. *Macromolecules* 29, 730-739.