**Supplementary Information**

**The effect of structure on solid state and subcooled liquid vapour pressures of organic isomers as measured with the Knudsen Effusion Mass Spectrometer**

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**Table S1. Subcooled vapour pressures found by using either Δcp,sl = 0 or Δcp,sl = ΔSfus. = ΔHfus/Tm and corresponding uncertainties for each compound.**





**Figure S1. Solid state vapour pressures for compound classes.**

**Spectra intensity determination**

Two methods were used to determine KEMS spectra intensities. KEMS studies (Booth et al. 2010, 2011; Krieger et al. 2018) have used a peak selection technique where the sum of peaks is added, and this is a proven method for finding vapour pressures. However integration of the KEMS spectra may also be an accurate method of analysis. To understand this, a subset of the 298K data presented here was analysed using both methods and the results are in Figure S2 with a 1:1 relationship plotted for reference.



**Figure S2. Vapour pressures found using both the integrating method and peak picking method for determining spectra intensities at 298K.**

**References**

Booth, A. M., M. H. Barley, D. O. Topping, G. McFiggans, A. Garforth, and C. J. Percival. 2010. Solid State and Sub-Cooled Liquid Vapour Pressures of Substituted Dicarboxylic Acids Using Knudsen Effusion Mass Spectrometry (KEMS) and Differential Scanning Calorimetry. *Atmos. Chem. Phys.* 10 (10): 4879–92. doi: 10.5194/acp-10-4879-2010.

Booth, A. M., W. J. Montague, M. H. Barley, D. O. Topping, G. McFiggans, A. Garforth, and C. J. Percival. 2011. Solid State and Sub-Cooled Liquid Vapour Pressures of Cyclic Aliphatic Dicarboxylic Acids. *Atmos. Chem. Phys.* 11 (2): 655–65. doi: 10.5194/acp-11-655-2011.

Krieger, U. K., F. Siegrist, C. Marcolli, E. U. Emanuelsson, F. M. Gøbel, M. Bilde, A. Marsh, J. P. Reid, A. J. Huisman, I. Riipinen, N. Hyttinen, N. Myllys, T. Kurtén, T. Bannan, C. J. Percival, and D. Topping. A Reference Data Set for Validating Vapor Pressure Measurement Techniques: Homologous Series of Polyethylene Glycols. *Atmos. Meas. Tech.* 11 (1): 49–63. doi: 10.5194/amt-11-49-2018.