Supporting Information

Isobaric Vapor-Liquid Equilibrium for Binary System of Isoamyl DL-Lactate + Isoamyl Alcohol at 25.0kPa, 50.0 kPa and 101.3 kPa

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The Concrete Calculating Process of Uncertainty Propagation

We show the concrete calculating process of uncertainty propagation in pressure.

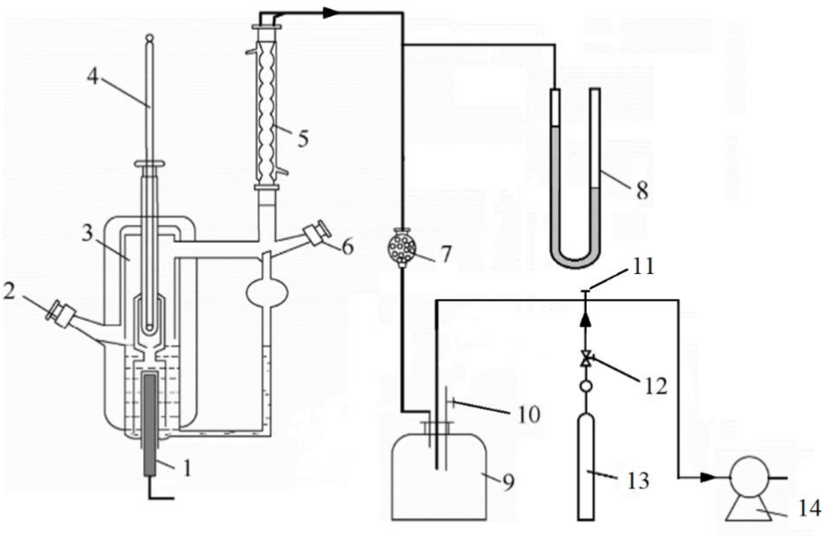

Figure S1. Schematic diagram of the experimental apparatus: (1) heating rod; (2) liquid-phase sampling port; (3) equilibrium chamber; (4) precision mercury thermometer; (5) condenser; (6) vapor-phase sampling port; (7) desiccator; (8) U-shaped mercury manometer; (9) pressure buffer tank; (10) needle valve; (11) three-port valve; (12) pressure relief valve; (13) nitrogen cylinder; (14) vacuum pump.

1. **Specification**

$$P = P_0 - \Delta P$$

Where

P_0: The local atmospheric pressure, kPa.

ΔP: The indicated value of the U-shaped mercury manometer, mmHg (≈0.133 kPa).

2. **Identifying and analyzing uncertainty sources**

The relevant uncertainty sources are shown in the cause and effect diagram as Figure S2.

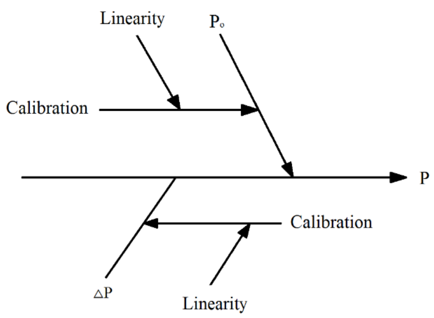

Figure S2. Cause and effect diagram

3. Calibration

3.1 The U-shaped manometer

① The U-shaped manometer has a maximum indicator value of 760 mmHg ± 1.0 mmHg at the temperature of 20 °C. The value of uncertainty is given without a confidence level or distribution information, so an assumption is necessary. Here, the standard uncertainty is calculated assuming a triangular distribution.

$$u_1(U-\text{shaped manometer}) = \frac{1.0\ mm\text{Hg}}{\sqrt{6}} = 0.408\ \text{mmHg}$$

② The temperature is 20 °C ± 2 °C in the laboratory (assumed to be uniformly distributed), and take the expansion coefficient of mercury ($1.8\times10^{-4}\,°C^{-1}$) as an example to calculate the influence of temperature (*T*) on U-shaped manometer, which can be expressed as:

$$u_2(T_{\text{U-shaped manometer}}) = \frac{760\times2\times1.8\times10^{-4}}{\sqrt{3}} = 0.158\ \text{mmHg}$$

Therefore, the uncertainty of the U-shaped manometer is:

$$u(\Delta P) = \sqrt{[u_1\ (U-\text{shaped manometer})]^2 + \left[u_2\left(T_{U-\text{shaped manometer}}\right)\right]^2} = 0.438 mm\text{Hg}$$

Convert mmHg to kPa:

$u(\Delta P) = 0.058\ \text{kPa}$

3.2 Atmospheric pressure gauge

The atmospheric pressure gauge manufacturer quotes ± 0.15 kPa for the linearity contribution. This value represents the maximum difference between the actual pressure and the measured pressure. The linearity contribution is assumed to show a rectangular distribution and is converted to a standard uncertainty:

$$u(P_0) = u(\text{Atmospheric pressure gauge}) = \frac{0.15\ \text{kPa}}{\sqrt{3}} = 0.087\ \text{kPa}$$

4. Calculating the combined standard uncertainty

P is given by

$$P = P_0 - \Delta P$$

The values of parameters in the above equation, their standard uncertainties are listed in Table S1.

Table S1. Uncertainties in composition analysis

	Description	Value	Standard uncertainty
ΔP	the maximum indicator value of U-shaped manometer	101.3 kPa	0.058 kPa
P_0	Atmospheric pressure	101.3 kPa	0.087 kPa

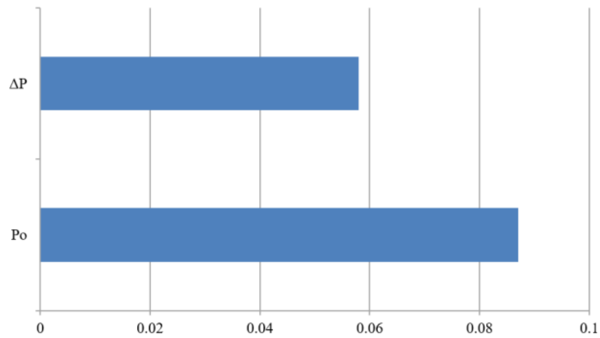

Figure S3. Uncertainty contributions

Using the values listed in Table S1:

$$u(P) = \sqrt{[u\ \ (\Delta P)]^2 + [u(P_0)]^2} = 0.104\ \ \text{kPa} \approx 0.1\ \ \text{kPa}$$

Therefore the standard uncertainties of pressure is about 0.1 kPa.

REFERENCES

(1) Ellison, S.L.R; Williams, A. Quantifying Uncertainty in Analytical Measurement, 3rd ed.; Eurachem, 2011

(2) Kirkup, L; Frenke, R. B. Guide to the expression of uncertainty in Measurement; 2006.