Supporting Information

Measurement and Correlation of Solubility of Tetramethylpyrazine in Nine Mono-Solvents and Two Binary Solvent Systems

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For method verification, the solubility of benzoic acid in ethanol, isopropyl alcohol and acetone at T = (288.15 to 298.15) K were re-measured by UV-Vis spectroscopy in this study at atmospheric pressure and compared with those data determined by the gravimetric method in the literature[1].
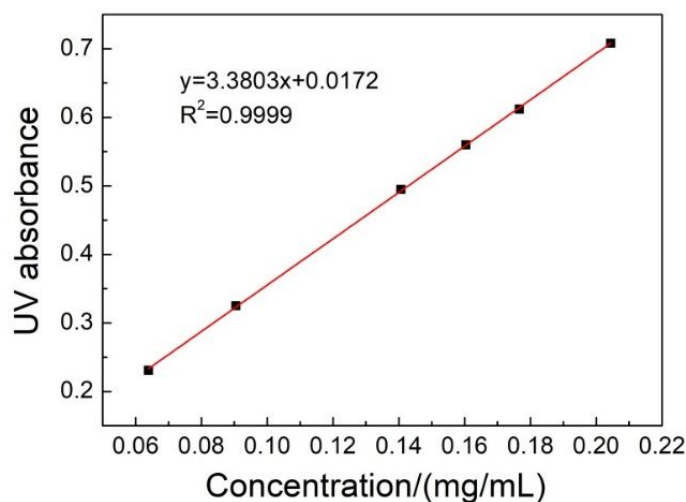

Fig.S1. Typical standard curve of absorbance *versus* solution concentration (mg·mL^{-1}) of benzoic acid for concentration determination at 283nm by UV-Vis spectroscopy

Table S1. Experimental mole fraction solubility (x^{exp}) of benzoic acid determined by UV-Vis spectroscopy in this study and those reported mole fraction solubility (x^{lit})[1] in ethanol, isopropyl alcohol and acetone at T = (288.15 to 298.15) K (P = 0.1 MPa).[a]

solvent	x^{exp}	x^{lit}	Deviation (%)
		T=288.15K	
ethanol	0.143	0.154	7.14
isopropyl alcohol	0.149	0.160	6.87
acetone	0.149	0.159	6.29
		T=293.15K	
ethanol	0.153	0.165	7.27
isopropyl alcohol	0.168	0.174	3.45

acetone	0.186	0.177	5.08

<div align="center">T=298.15K</div>

ethanol	0.168	0.178	5.62
isopropyl alcohol	0.182	0.193	5.70
acetone	0.208	0.197	5.58

[a] The standard uncertainty of T is $u(T) = 0.1$ K. The relative standard uncertainty of the solubility is $u_r(x) = 0.05$. The relative uncertainty of pressure is $u_r(P) = 0.05$.

From the table, it is obvious that the deviation is no more than 7.27%, indicating the method used in this study is creditable and reliable. The deviation may be caused by the instrumental error, measurement methods and other errors. The instrumental error is determined by the instrumental accuracy. For example, the accuracy of an electric balance is ± 0.0001 g, the accuracy of a shaker is ± 0.1 K, all of these could bring about the instrument error. In addition, the measurement error may be resulted from experimental operations such as weighing and sampling.

References:

1. Sandeepa, K.; Ravi Kumar, K.; Neeharika, T. S.; Satyavathi, B.; Thella, P. K. Solubility Measurement and Thermodynamic Modeling of Benzoic Acid in Monosolvents and Binary Mixtures. *J. Chem. Eng. Data* **2018**, 63, 2028−2037.