PCCP



CORRECTION

View Article Online



Cite this: Phys. Chem. Chem. Phys., 2019, 21, 12704

Correction: Maxwell—Stefan diffusion coefficient estimation for ternary systems: an ideal ternary alcohol system

Tariq Allie-Ebrahim, Qingyu Zhu, Pierre Bräuer, Geoff D. Moggridge and Carmine D'Agostino*†

DOI: 10.1039/c9cp90142f

rsc.li/pccp

Correction for 'Maxwell-Stefan diffusion coefficient estimation for ternary systems: an ideal ternary alcohol system' by Tariq Allie-Ebrahim et al., Phys. Chem. Chem. Phys., 2017, 19, 16071–16077.

There was a typographical error in the originally published manuscript. The error originates in Table 1, the values in which were used to calculate Table 2. The values given in the originally published version of Table 1 cannot be used to satisfactorily fit the VLE data given in the references; and indeed cannot be used to obtain the values which were published in Table 2. Following re-calculation of the binary NRTL parameters, obtained by a least squares fit to the binary VLE data sets, a revised Table 1 is given below.

From this revised Table 1, a new Table 2 (shown below) was also calculated. The values in the revised Table 2 are very similar to those in the original Table 2, and therefore the key conclusion that all mixtures are very close to ideal holds. Thus, the discussion and conclusions of the paper remain unaltered.

Table 1 Regressed ternary NRTL parameters for methanol (1)/butan-1-ol (2)/propan-1-ol (3) at 298 K i–j τ_{i-j} α 1-2 1 0814 -0.71050.3 1-3 1.1651 -0.81660.3 2-3 0.0491 -0.01380.3

Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS, UK

[†] Current address: School of Chemical Engineering and Analytical Science, The University of Manchester, The Mill, Sackville Street, Manchester, M1 3AL, UK. E-mail: carmine.dagostino@manchester.ac.uk

Correction

Table 2 Calculated thermodynamic correction factor matrix, Γ , for methanol (1)/butan-1-ol (2)/propan-1-ol (3) using the regressed ternary NRTL parameters for the eight mixtures investigated

Exp.	x_1	x_2	x_3	Γ	
1	0.9	0.05	0.05	0.9564 0.0227	0.0080 0.9932
2	0.1	0.45	0.45	1.0075 0.0037	0.0062 0.9804
3	0.45	0.1	0.45	0.9891 0.0057	0.0150 0.9902
4	0.45	0.45	0.1	0.9838 0.0156	0.0247 0.9726
5	0.6	0.1	0.3	$0.9648 \\ 0.0120$	0.0158 0.9890
6	0.1	0.6	0.3	1.0072 0.0007	0.0069 0.9807
7	0.3	0.1	0.6	1.0061 0.0031	0.0120 0.9915
8	0.333	0.333	0.334	1.0005 0.0057	0.0170 0.9779

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.