Reply to Comments by García, Alcalde, Aparicio, Dávila, Leal, and Matos on J. Chem. Eng. Data 2004, 49, 235–242

Nandhibatla V. Sastry

Physical Chemistry 1, University of Bayreuth, D-95440 Bayreuth, Germany

1. Correction. There is an error in Figure 3 a and b. The literature $V_{\rm m}^{\rm E}$ values (from ref 8) were incorrectly and inadvertently calculated by a confusion in swapping the amide mole fractions to water and vice versa. This lead to the incorrect statement on previous data published by Garcia et al.⁸ The revised Figure 3 along with the correct literature values is reproduced below. For the sake of clarity, we have shown only our smoothed $V_{\rm m}^{\rm E}$ values for the two mixtures. Accordingly, lines 19–21 of the second column on page 238 should be read as "The literature values from Garcia et al.⁸ for the 2-pyrrolidinone, + 1-methyl-2-pyrrolidinone + water mixtures at T = 298.15 K, however, matched very well with our values for the same mixtures and at the same temperature."

2. The GC purities of our chemicals (PYR, NMP) are \sim 99% and >99% with free amine content of 0.01% and water content <0.002% (from Karl Fischer titration). Thus, we subjected the chemicals to fractional distillation, and only the middle fractions are collected and employed in the work.

3. We are exploring the ways and means to get the automatic calibration procedure using liquid standards other than water and at prior selected temperatures for our Paar DMA 5000 density meter.

4. The sixth digit in the densities of pure and mixture components in Tables 1 and 2 is shown separately to indicate uncertainty limits. It may be noted that $V_{\rm m}^{\rm E}$ values are given only up to three significant digits after the decimal. The reported density values have an uncertainty of better than 3×10^{-6} g·cm⁻³, and hence six-digit density values with last digit given after a space are justified.

5. To handle the measurements of dynamic viscosities ranging from 0.438 to 13.363 mPa·s, we have employed three separate viscometers with capillary bores of 0.5, 0.7, and 1 mm. The capillary tube has a length of about 8.5 cm, and the flow volumes varied from 110 to 310 s for minimum and maximum viscosities. Hence, we believe that drainage and shear corrections are sufficiently taken care of. Yes, we agree that viscometers other than the capillary type would give more accurate results.

Received for Review October 8, 2004. Accepted October 19, 2004. JE0496443



Figure 3. Variation of excess molar volumes, V_{m}^{E} , with the water mole fraction for the representative binary mixtures: (a) water + 2-pyrrolidinone at different temperatures. Curves represent smoothed values using eq 3 and coefficients from Table 6. Curves 1, 2, 3, 4, and 5 are at T = (298.15, 308.15, 318.15, 328.15, and 338.15) K. Literature values are at T = 298.15 K (+, ref 8; \bullet , ref 10; \Box , ref 5), at T = 308.15 K (\bullet , ref 10; \times , ref 5), and at T = 318.15 K (\blacksquare , ref 5). (b) Water l-methyl-2-pyrrolidinone. Curves are the same as for water + 2- pyrrolidinone. Literature values are at T = 298.15 K (+, ref 8; \bullet , ref 10) and at T = 308.15 K (\Box , ref 10).