

COMMENTARY ON “STUDIES ON MOLAR VOLUME, DIELECTRIC PROPERTIES AND REFRACTIVE INDICES OF CYANEX 923 + BENZENE/XYLENE AT 300 K”

William E. Acree, Jr.

Department of Chemistry, University of North Texas, 1155 Union Circle Drive #305070, Denton, TX 76203 (USA)

Abstract

Redlich-Kister equation coefficients reported by Satpathy and coworkers [J. Mol. Liq. 222 (2016) 383-389] for binary benzene + cyanex 923 and xylene + cyanex 923 are found to be inconsistent with the graphs of the experimental excess molar volumes, excess molar polarizabilities and excess molar refractions. Values calculated from the reported Redlich-Kister equation coefficients differ significantly from the measured experimental data.

Key Words and Phrases:

Excess molar volumes; Molar refractions; Molar polarizabilities; Cyanex 923; Redlich-Kister mathematical representation

*To whom correspondence should be addressed. (E-mail: acree@unt.edu); fax: 940-565-4318.

In a recent paper published in *This Journal* Satpathy and coworkers [1] reported the experimental densities, dielectric constants and refractive indices of binary mixtures of benzene (1) + Cyanex 923 (2) and xylene (1) + Cyanex 923 (2). Measurements were performed at only a single temperature of $T = 300$ K, and over the entire mole fraction concentration range. Experimental values for benzene and xylene were not included in the published tables of experimental data, and the specific xylene isomer studied was not identified. The measured experimental values were used to calculate the molar volumes, molar polarizations and molar refractions. The authors calculated the excess parameters, assuming mole fraction additivity:

$$A^E = A_{12} - (X_1 A_1 + X_2 A_2) \quad (1)$$

where A_{12} is the given property for the binary mixture, and X_i and A_i represent the mole fraction and the given property of component i in the mixture. The excess quantities were then mathematically described using the Redlich-Kister polynomial equation:

$$A^E = X_2 (1 - X_2) [a_0 + a_1 (2 X_2 - 1) + a_2 (2 X_2 - 1)^2 + a_3 (2 X_2 - 1)^3] \quad (2)$$

Numerical values of the four curve-fit coefficients (a_0 , a_1 , a_2 and a_3) can be determined through regression analyses of the excess values in accordance with Eqn. 2.

The purpose of this brief commentary is to inform journal readers that the authors' published Redlich-Kister equation coefficients, given in Tables 2 and 3 of their published paper [1], do not describe the excess values that are graphically depicted in Figures 2, 5 and 6. The inconsistencies between the coefficients and graphs can be quickly shown by calculating the numerical of A^E at $X_2 = 0.5$, where only the a_0 coefficient contributes to the Redlich-Kister computation. For the excess molar volume computations, I calculate $V^E = -0.558 \times 0.25 = -0.14$ cm³/mole (benzene + Cyanex 923) and $V^E = 0.25 \times 2.365 = 0.59$ cm³/mole (xylene + Cyanex 923), which differ significantly from the values of $V^E = 1.2$ cm³/mole and $V^E = 4.0$ cm³/mole that are

obtained from Figure 2. Similarly, I calculate $P^E = 0.25 \times 16.44 = 4.11 \text{ cm}^3/\text{mole}$ (benzene + Cyanex 923) and $P^E = 0.25 \times 13.85 = 3.46 \text{ cm}^3/\text{mole}$ (xylene + Cyanex 923) at $X_2 = 0.5$. Figure 5 in the published paper shows the values to be negative for both mixtures. The numerical values taken from the figure are on the order $P^E = -60 \text{ cm}^3/\text{mole}$. I have assumed the units to be cm^3/mole which is consistent with how the values are given in Table 1 of the paper by Satpathy et al. The manuscript text also states that the values of P^E are negative; however positive numerical values are calculated using the authors' tabulated Redlich-Kister coefficients from Tables 2 and 3. There are clearly inconsistencies between the tabulated coefficients and the figures in the published paper of Satpathy et al.

References

- [1] S. Satpathy, S. Pradhan, S. Mishra, J. Mol. Liq. 222 (2016) 383.

HIGHLIGHTS

- Published Redlich-Kister coefficients for excess volumes inconsistent with graphs of experimental data
- Published Redlich-Kister coefficients for excess molar refractions inconsistent with graphs of experimental data
- Published Redlich-Kister coefficients for excess molar polarizations inconsistent with graphs of experimental data