

Prediction of Dielectric Constants of (Cyclic Ketone- 1,4-Butanediol) Binary Systems

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ABSTRACT

In order to predict the permittivity and excess permittivity data of binary systems containing cyclic ketones (cyclohexanone and cyclopentanone) and 1,4-butanediols, various mixing rules were used [1,2]. The permittivity increment, $\Delta\epsilon = \epsilon_{12} - (x_1\epsilon_1 + x_2\epsilon_2)$, was also evaluated in this research using the predicted data. x_1 and x_2 are the mole fractions of the components 1 and 2, ϵ_1 and ϵ_2 are the permittivities of the pure components. As shown in Fig. 1, the experimental permittivity values for three systems containing 1,4-butanediol (1,4BD) and two cyclic ketones were estimated by several mixing rules. Typically, for cyclohexanone and 1,4-butanediol mixtures, the predicted excess permittivity data were compared and shown in Fig. 2. As it can be seen from Table 1, the Lichteneker-Rother model shows the lower root mean square deviation (rmsd) value, which indicates that the Lichteneker-Rother model presents the best result between the predictive models.

Keywords: Cyclic Ketone- 1,4-Butanediol, Binary Systems

Table 1

Standard deviations of the experimental permittivity from those estimated by mixing rules for the binary mixtures.

| Mixing rules | 1,4BD + CHO | 1,4BD + CPO |
|----------------------|-------------|-------------|
| | RMSD | RMSD |
| Looyenga | 0.53 | 0.14 |
| Bottcher-Bordewijk | 0.52 | 0.10 |
| Bruggeman asymmetric | 0.59 | 0.09 |
| Peon-Iglesias | 0.52 | 0.18 |
| Iglesias-Peon | 0.51 | 0.19 |
| Lichteneker-Rother | 0.27 | 0.53 |
| Kraszewski | 0.67 | 0.16 |
| H.S.Upper bound | 0.40 | 0.38 |
| Brown | 0.52 | 0.10 |
| Rayleigh-Maxwell | 0.65 | 0.17 |
| Onsager-Botcher | 0.52 | 0.10 |
| Iglesias | 0.93 | 0.49 |
| Grosse-Grefe | 0.60 | 0.13 |
| Sen | 0.46 | 0.24 |

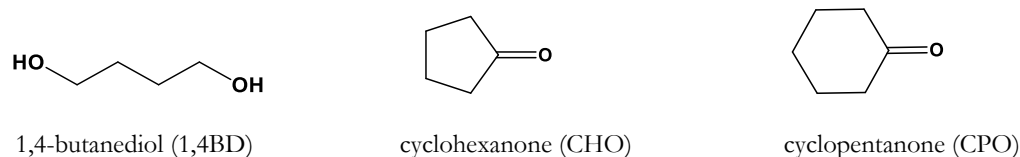


Figure 1. Chemical structures of the used compounds

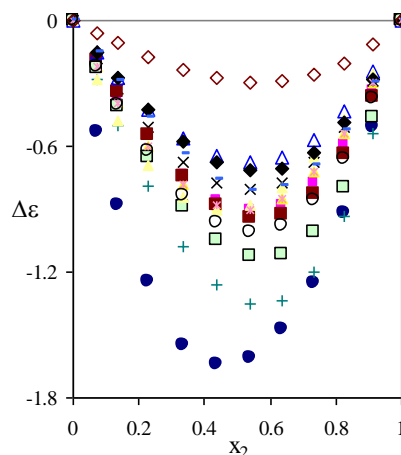


Figure 2. Predicted permittivity increments for binary mixtures of [CHO (1) + 1,4BD (2)] at $T = 298.2$:

Reference

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