

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

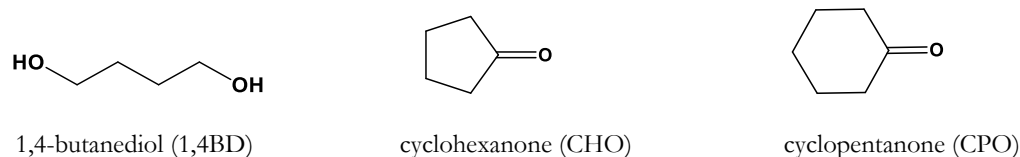


Figure 1. Chemical structures of the used compounds

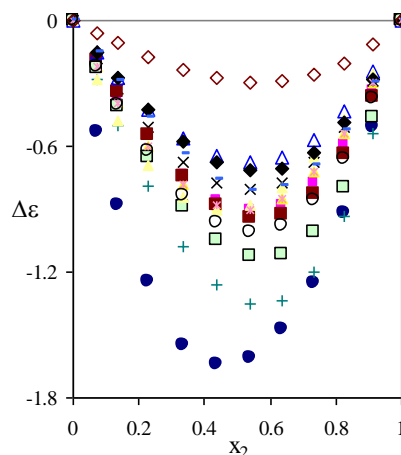


Figure 2. Predicted permittivity increments for binary mixtures of [CHO (1) + 1,4BD (2)] at $T = 298.2$:

Reference

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