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Brief Communication

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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, $\Delta\varepsilon = \varepsilon_{12} - (x_1\varepsilon_1 + x_2\varepsilon_2)$, 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.

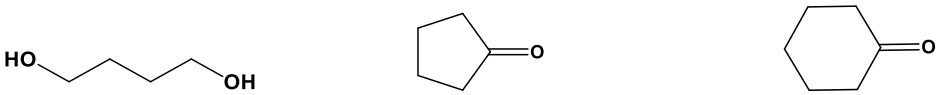
	1,4BD + CHO	1,4BD + CPO
Mixing rules	**RMSD**	**RMSD**
Looyenga	0.53	0.14
Bottcher-Bordewijk	0.52	0.10
Bruggeman asymmetric	0.59	0.09
Peon-Iglesias	0.52	0.18
Iglesias-Peon	0.51	0.19
Lichteneker-Rother	0.27	0.53
Kraszewski	0.67	0.16
H.S.Upper bound	0.40	0.38
Brown	0.52	0.10
Rayleight-Maxwell	0.65	0.17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

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1,4-butanediol (1,4BD) cyclohexanone (CHO) cyclopentanone (CPO)

Figure 1. Chemical structures of the used compounds

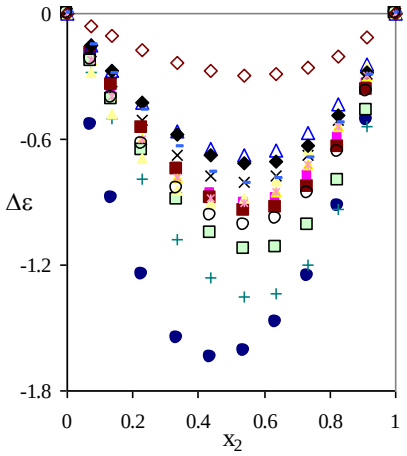


Figure 2. Predicted permittivity increments for binary mixtures of [CHO (1) + 1,4BD (2)] at T = 298.2:

Reference

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2. Gupta H, Chandrasekhar M, Krishna TS, Sharma VK. *J Mol Liq*. 2017; 231: 225-237.

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