





ALKHAS, 2021; 3(1): 18-19

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

Zahra Mohammadalipoor and Ali Ghanadzadeh Gilani*



Department of Chemistry, Faculty of Science, University of Guilan, Rasht, Iran.

*Corresponding Author:



Received: 15 December, 2020 Accepted: 10 January, 2021 Published: 30 January, 2021

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 1Standard deviations of the experimental permittivity from those estimated by mixing rules for the binary mixtures.

those estimated by illians	1,4BD + CHO	
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



Publisher: Scientific Research Publishing House (SRPH), Shirvan, Iran

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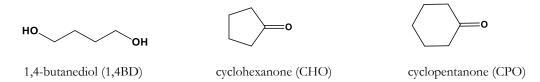


Figure 1. Chemical structures of the used compounds

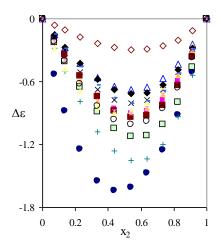


Figure 2. Predicted permittivity increments for binary mixtures of [CHO (1) + 1,4BD (2)] at T = 298.2:

Reference

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Citation: Mohammadalipoor Z, Ghanadzadeh Gilani A. Prediction of Dielectric Constants of (Cyclic Ketone- 1,4-Butanediol) Binary Systems. ALKHAS. 2021; 3(1): 18-19.

https://doi.org/10.47176/alkhass.3.1.18