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Excess Thermodynamic Properties of Binary Liquid Mixtures of Butanol Isomers with Di-n-Butyl Ether at 298.15 K, 0.1 MPa

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Binary liquid mixtures of alcohols and ethers are of importance as potential biofuels or additives for internal combustion engines,[1] and have also attracted fundamental interest as model liquid systems containing one component (the alcohol) that can strongly self-associate through hydrogen bonding (HB), and one that cannot self-associate via HBs (ether), yet can interact strongly with the former as HB acceptor.[2] The excess thermodynamic properties of these mixtures, specifically the excess molar enthalpies and volumes (HE and VE), have been extensively measured.[1-3] Butanol isomer + di-*n*-butyl ether (DBE) binary mixtures, in particular, show interesting volumetric differences, with VE changing from negative (1- and *iso*-butanol) to positive (2- and *tert*-butanol) with increasing butanol alkyl group branching. Representative 1- and 2-butanol + DBE mixtures were studied, for the first time, by atomic-resolution classical Molecular Dynamics (MD) computer simulations. The simulations reveal decided differences in the degree of self-association of the two butanol isomers and support existing interpretations of the HE and VE in a general sense, but also suggest that more subtle differences in H-bonded topologies may contribute significantly to the anomalous volumetric properties of these mixtures.[4]
<img src="https://indico.bitp.kiev.ua/event/7/contributions/199/attachments/80/151/Fig1_L Engelbrecht.jpg" >

$Fig. 1. MD computer simulation configurations of equimolar mixtures of 1-or 2-butanol with DBE. Ethermoleculesareomitt$
$filling(redandwhitespheres)representationinordertohighlightthedifferencesinHBtopologies.Simulationcelledgesaresho$

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Primary author: ENGELBRECHT, Leon (University of Cagliari, Italy)

Presenter: ENGELBRECHT, Leon (University of Cagliari, Italy)

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