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## Water activity in polyol/water systems: new UNIFAC parameterization

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**Abstract.** Water activities of a series of polyol/water systems were measured with an AquaLab dew point water activity meter at 298K. The investigated polyols with carbon numbers from  $n=2-7$  are all in liquid state at room temperature and miscible at any molar ratio with water. In aqueous solutions with the same molar concentration, the diols with lower molecular weight lead to lower water activities than those with higher molecular weights. For diols with four or more carbon atoms, the hydrophilicity shows considerable differences between isomers: The 1,2-isomers - consisting of a hydrophilic and a hydrophobic part - bind less strongly to water than isomers with a more balanced distribution of the hydroxyl groups. The experimental water activities were compared with the predictions of the group contribution method UNIFAC: the model predictions overestimate the water activity of water/polyol systems of substances with two or more hydroxyl groups and can not describe the decreased binding to water of isomers with hydrophobic tails. To account for the differences between isomers, a modified UNIFAC parameterization was developed, that allows to discriminate between three types of alkyl groups depending on their position in the molecule. These new group interaction parameters were calculated using water activities of alcohol/water mixtures. This leads to a distinctly improved agreement of model predictions with experimental results while largely keeping the simplicity of the functional group approach.

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