N-Hexanol association in cyclohexane studied by NMR and NIR spectroscopies

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In this work we present a study on the association of n-hexanol in cyclohexane using NMR and NIR spectroscopies. Abrupt changes on spectroscopic responses have been observed at low molar fractions of n-hexanol, which are related to hydrogen bond network formation that includes trace water. Molecular interactions are found to be dominated by dispersion forces, hydrogen bonding, and dipolar interactions, to different extents at different n-hexanol composition ranges. 1D, DOSY, and T_1 and T_2 relaxation time analyses by 1H-NMR allow understanding the dynamics of the mixtures. NIR allows verifying the formation of n-hexanol polymeric species. In addition, an n-hexanol/cyclohexane mixture with an alcohol molar fraction of 0.177 has been titrated with water, revealing the formation of a microemulsion containing water droplets that evolves to a bicontinuous microemulsion with increasing water content. Stable boundary water is detected at the microemulsion interface. © 2014 Elsevier B.V.

Alcohol self-association

NIR

NMR

Water-in-oil microemulsions

N-hexanol

NIR

NIR spectroscopy

Self-associations

Water-in-oil microemulsions

Nuclear magnetic resonance