Solvent Strength Effects on the Antisolvent Ability of CO_2 with Organic/IL Mixtures

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Ionic Liquids (ILs) have been successfully used as solvents for various reactions, but the separation of products and catalysts remains an issue. Previously, our group has shown that CO_2 can induce a liquid-liquid phase split with IL/organic mixtures [1], extract solid solutes from ILs [2], and precipitate solid solutes from IL/organic mixtures [3]. Here we investigate the effects of different organics to understand the specific interactions that dominate IL/organic mixtures. The lower critical endpoint (LCEP), the CO_2 pressure required to induce a liquid-liquid phase split, is one measure of the antisolvent ability of CO_2. We complement this with measurements of the solvent strength of IL/organic/CO_2 mixtures using spectroscopic probes. Previously, we used the Kamlet-Taft parameters to show that the solvent strength of ILs are not influenced by CO_2, even at high pressures [4]. Here, we expand upon our previous work to understand the solvent strength of binary and ternary mixtures of ILs with high pressure CO_2. In particular, we present Kamlet-Taft parameters for organic/IL, IL/CO_2, and organic/IL/CO_2 systems. In addition, the solvatochromic probe Acetylacetonato-N,N,N',N'-tetramethylethylenediaminocopper(II) tetraphenylborate ([Cu(acac)(tmen)][BPh_4]) has a structure similar to that of organometallic catalysts. We use CO_2 to precipitate this probe from IL/organic mixtures, while examining the effects of the solvent strength at the same conditions. The ultimate goal is to develop a correlation between the solvent strength and the antisolvent ability of CO_2 to allow for the selection and design of IL/CO_2 systems for reactions, as well as for product and catalyst separations.

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