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Separation and Phase Behavior of Double-Decker Silsesquioxane Isomers

Andre Lee
Dept. of Chemical Engineering and Materials Science
Michigan State University

By virtue of regio- and geometric isomers, functionalized double-decker silsesquioxanes (DDSQ) may offer unique access to silsesquioxane-based hybrid materials with multifaceted performance characteristics. Analytical methods were as used to separate cis and trans isomers of various DDSQ with polar as well as nonpolar moieties. Solubility was fitted to the Schröder-van Laar equation with activity coefficients determined using the NRTL model by adjusting binary interaction parameters. For a given DDSQ compound, the variances in solubility between cis and trans isomers depend on differences in thermal properties. cis and trans isomers binary phase diagrams of DDSQs were also developed to examine the influence of the regioisomer (meta- or para-) and the nonactive organic moiety coupled on the D-silicon. DDSQ compounds with a methyl moiety exhibited eutectic phase diagrams. Their trans isomers were higher melting and exhibited larger packing density. Cyclohexyl DDSQ exhibited an isomorphic phase diagram, attributed to cyclohexyl being more similar in size to the phenyl moieties. Changing from para- to meta-aminophenyl shifted the solid-liquid equilibrium further from ideal, with decreased activity coefficients.