ABSTRACT

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Solubility and Partitioning of C_{60}. Major Professor: Chad Jafvert.

The potential large scale production of fullerene C_{60} and its widespread use in consumer products may translate into occupational and public exposure and in long term environmental exposure. In this study, the solubility of C_{60} was measured in mixtures of toluene-acetonitrile, toluene-ethanol, toluene-tetrahydrofuran, and acetonitrile-tetrahydrofuran and the solubility data were modeled using Wohl's equation. The estimated crystal energy term for C_{60} in tetrahydrofuran was different than that in the other solvents indicating that C_{60} may form solvates in tetrahydrofuran.

The log K_{ow} of C_{60} was measured to be 6.67, and the toluene-water partition coefficient was measured at log K_{tw} = 8.44. From these values and the respective solubilities of C_{60} in water-saturated octanol and water-saturated toluene, C_{60}'s aqueous solubility was calculated to be 7.96 ng/L. Because it is widely known that clusters form in aqueous solutions upon mixing crystalline C_{60} with water, this value can be regarded as the hypothetical solubility in water, as the activity of C_{60} in water at this concentration will result in the more thermodynamically favorable clusters in which C_{60} has a lower activity, resulting in an associated lower dissolved aqueous concentration of molecular C_{60} at equilibrium. Additionally, solubility of C_{60} was measured in mixtures of ethanol-water and tetrahydrofuran-water and modeled with Wohl's equation, to confirm the accuracy of the "hypothetical" solubility value. Results of a generator column experiment strongly support the notion that clusters form at aqueous concentrations below the solubility limit. The K_{ow} value is compared to those of other hydrophobic organic compounds such as *p,p'*-DDT, and bioconcentration factors for C_{60} were estimated based on K_{ow}.

Additionally, some widely used solubility models, their assumptions, and accuracy for predicting solubility of C_{60} and PAHs are discussed. Solubility data for naphthalene, phenanthrene, pyrene, and perylene in alcohol-water mixtures were compared with predicted solubilities using the log-linear cosolvency model and the Wohl's equation. The interaction parameters in Wohl's equation were regressed against each solutes log K_{ow} and the relationship was used to estimate interaction parameters and solubility of similar PAHs in alcohol-water mixtures. Further, the model was extended to predict solubility of C_{60} in ethanol-water and propanol-water mixtures.