

## Aqueous Solubility of Hydrocarbons as a Function of Molecular Structure

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The prediction of the transport and fate of hydrocarbons in the environment requires the knowledge of their physical and chemical properties. An important quantity is the solubility in water which in combination with vapor pressures allows to calculate the Henry's law constant related to different partition coefficients such as the air/water or octanol/water partition coefficients. The solubility is of capital importance for environmental processes affecting adsorption and desorption in soils, volatility of chemicals from aquatic systems, chemical reactions such as hydrolysis, photolysis or biodegradation and other specialized pathways like the washout from atmosphere by rain. In the present work, original experimental results of the water solubility of several hydrocarbons are reported as a function of temperature between 0 and 45°C. The hydrocarbons studied all contain eight carbon atoms and they differ in their molecular structure. The objective was to examine how these differences influence their solubility in water. Several features were assessed: the effect of cycling (cyclooctane); the presence of a double bond (cyclooctene); the influence of different substitutes on a cyclohexane ring (ethylcyclohexane, cis- and trans-1,2-dimethylcyclohexane) and the effect of the branching of the aliphatic chain (2,5-dimethylhexane and 2,2-dimethylhexane). The differences in water solubility were important enough to be detectable given the precision of measurements. It was observed that cyclooctane was significantly more soluble in water than octane and that the presence of a double bond further increases the solubility. Concerning the effect of substitution on the cyclohexane ring, the solubility is slightly higher for cis-1,2-dimethylcyclohexane than for the trans isomer, both dimethylcyclohexanes being more soluble than ethylcyclohexane. The branching of the aliphatic chain increases significantly the solubility. The Henry's law constants were calculated using the recommended vapor pressure data from literature. The apparatus used is based on the dynamic saturation column method and was designed for the measurement of solubilities between 10<sup>-6</sup> and 10<sup>-10</sup> in molar fraction. The first step of the experimental determination consists in the saturation of a known quantity of water with an organic solute and its subsequent capture in a specific extraction cell. The second step involves the extraction of the solute by an appropriate organic solvent. This final solution is then analysed by gas chromatography. The experimental technique was validated by the study of n-octane in water from 10 to 45°C and the results, expressed as molar fraction solubilities, exhibit an imprecision of ±5% and an estimated accuracy of ±10%.