

Correlations of the Solubility of Gases in Liquids

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The solubility of gases in liquids is important both for theoretical and practical reasons. We have gathered into three data bases the following information: (1) gas solubility data in terms of mole fraction at 1 atm partial pressure of gas and 298.15 K (x_2); (2) physical properties of over 150 gases; and (3) physical properties of over 150 solvents. Using the programs QSARIS, SAS, and SigmaPlot, we have engaged in a systematic study searching for the best correlations between $\ln x_2$ and properties of the gases and solvents. We have carried out factor analysis studies, and will report the results. Generally, no more than two factors are required for adequate correlations (R^2 of 0.9 or better). We have used both experimentally based physical properties and calculated descriptors in our work. The latter are quite useful, since they can be generated by various programs from the structure of the molecule. Since polarizability is an important factor, we have carried out a separate study to arrive at the best set of these values, and this will be reported. The initial ambition was to find one equation to cover all of the systems. This was not possible, and results will be given for correlations determined for classes of compounds. Water is a unique solvent, and is treated separately. We have also worked out a method to correlate solubility with properties of both the solute and the solvent -- this will be discussed. Following completion of the studies, our data bases will be made freely available.