

Solvation Thermodynamics Quantities for Pure Fluids

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Solvation thermodynamic quantities are essential in both characterization and interpretation of any process carried out in the liquid phase. In this talk we will describe our efforts to derive solvation thermodynamic quantities from data found in the NIST REFPROP database. The NIST REFPROP database implements the most accurate pure fluid models currently available and we expect that the present results, derived from REFPROP, are of similarly high quality and thus represent one of the best and most consistent sets of solvation thermodynamics data currently available. Using the standard definition of the solvation process, we have derived solvation thermodynamics quantities of a molecule in its own fluid for 76 pure fluids found in the REFPROP database. These results will be presented and compared to the best-available experimental values for selected molecules. Full results for all 76 pure fluids will be available in a NIST Special Publication. We expect these data to be valuable for comparing to similar experimental data, for making computation which require solvation thermodynamic quantities, and for developing new theoretical models designed to compute solvation thermodynamic quantities. The work on pure fluids represents the first phase of this project. Recent work on aqueous solutions will also be discussed.