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CURRENT RESEARCH

EXPERIMENTAL AND THEORETICAL APPROACHES TO THE PROPERTIES OF HIGH TEMPERATURE AQUEOUS SOLUTIONS: Our interest in aqueous solutions at high temperatures is motivated by the role they play in such process as mineral transport and deposition, hydrocarbon accumulation, electric-power-boiler corrosion, and the utilization of hydrothermal reservoirs. The long-term goal is understanding prediction of solution properties.

On the experimental side, instruments have been developed to make more accurate and rapid measurements of the heat capacities and densities of aqueous solutions at temperatures to 425 C and pressures to 350 atmospheres (atm). The instruments are unique and allow us to explore the spectacularly large effects of adding solutes on heat capacities and volumes of solutions near the critical point of water. More recently, we have developed instruments for measuring conductance in this temperature range. All salts are weak electrolytes at these temperatures and the conductance measurements allow us to measure their association equilibria. These association reactions have a large effect on water-rock equilibria.

SIMULATIONS. In order to understand our natural environment, geochemists need to know the properties of aqueous solutions at the extremes of temperature and pressure at which they occur (at least to 1200 C and 10,000 atm). It is too time-consuming to do experiments on all possible natural species, so it is important to develop predictions.

We first construct approximate models of forces in aqueous solutions in order to predict by computer simulation the properties of very high temperature aqueous solutions (to 1200 C and 10,000 atm). We then calculate trajectories of about



250 molecules. The temperature and pressure of the simulation are easily adjusted. Finally, we calculate all the thermodynamic properties of this model.

Then, in collaboration with Prof. Doren, we are using quantum mechanics to calculate the difference between our approximately models and accurate quantum models. Thus we calculate free energies and structures of our accurate quantum models.

REPRESENTATIVE PUBLICATIONS

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S. Sakane, E. M. Yezdimer, W. Liu, J. A. Barriocanal, D. J. Doren and R. H. Wood, Exploring the ab initio/Classical Free Energy Perturbation Method: The Hydration Free Energy of Water," *J. Chem. Phys.* (2000) 113, 2583-2593.

A. V. Plyasunov, J. P. O'Connell, R. H. Wood and E. L. Shock, "Infinite Dilution Partial Molar Properties of Aqueous Solutions of Nonelectrolytes. II. Equations for the Standard Thermodynamic Functions of Hydration of Volatile Nonelectrolytes over Wide Ranges of Conditions including the Subcritical Temperatures," *Geochim. Cosmochim. Acta* (2000) 64, 2779-2795.

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