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Alan Tomlinson
Principal Inversigator
Coalloid Engine Co.

30th October 1992

Dear Alan,

I hope that the following collection of thoughts is helpful. I feel that a list of recommendations is now required and that this list should be composed after consultation with you.

Regards

Wayne Davies

**Supercritical Water - A Review, Report and Collection of Thoughts
for Coalloid Engine Company**

Thoughts on Structure and Solvent Properties

Ordinary water can be thought of as an extended molecular network. The molecules of H₂O represent the simplest but not very structural formula for water. As a liquid this material is really a large macromolecule held together by hydrogen bonds i.e. (H₂O)_n where n can be a large number (100 or so) which tends to increase as the temperature drops and vice versa. The macromolecules of liquid water is not constant however and the individual H₂O's which make them up do not remain with the same macromolecule but exchange with their neighbours at high frequency. This is reason for the use of the term "flickering clusters". The dipole moment of water is high owing to the bond angle of the hydrogen-oxygen-hydrogen configuration which is less than 180 degrees. Electrons attracted to the oxygen make it slightly negative leaving the hydrogens slightly positive. This imbalance of charges gives rise to "hydrogen bonding" i.e. the attraction of adjacent oxygens to hydrogens of a different water molecule. The extended network of these hydrogen bonds gives the unique properties of water that we are aware of, i.e. high boiling point, relatively high viscosity, good solvent properties for polar materials etc. Water's ability to dissolve ionic species is more a function of the dissociation of ions and their hydration by water than its hydrogen bonding ability.

As the gas, water molecules are effectively in a monomolecular state. The distances between them are too large to allow hydrogen bonding and their kinetic energy is too great to allow molecular interactions to form larger molecules. The dipole moment is still quite high for the same reasons that it is in liquid water, i.e. the bond angle and the electronegativity of the oxygen compared to the hydrogen.

