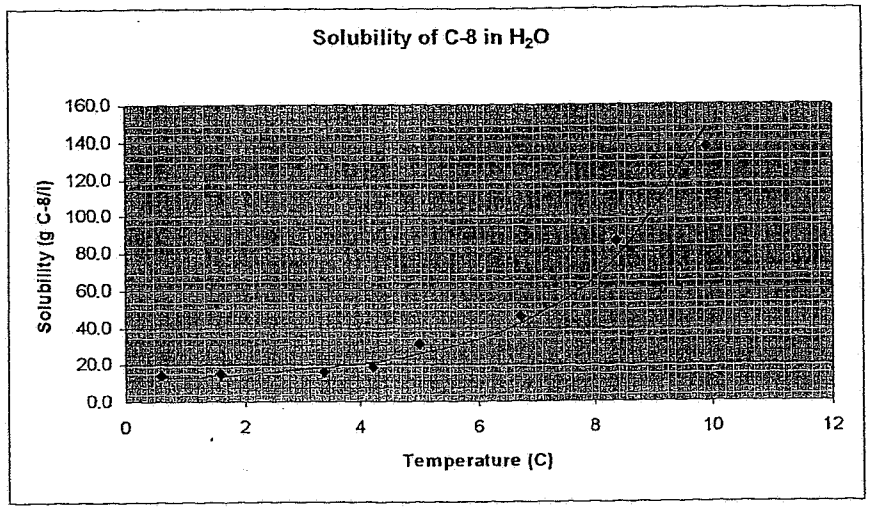
Solubility of C-8 in Water and General Effect of pH

The solubility of C-8 in water has been studied and published in the open literature by Shinoda (Shinoda, K., et al, J. Phys. Chem., V 76, No. 6 (1972)). Data have been collected at low temperatures (<10°C), which extend slightly above the Krafft point. The Krafft point is defined as the temperature at which the solubility of an ionic surfactant becomes equal to the Critical Micelle Concentration (CMC), and is equal to 2.5°C for C-8. The CMC is equal to 0.033 mole/liter. These data are shown below in tabular and graphical form.

Temp	Solubility	Solubility
C	mol/l	g C-8/l
0.6	0.0326	14.0506
1.58	0.0339	14.6109
3.4	0.0367	15.8177
4.24	0.0438	18.8778
5.01	0.0716	30.8596
6.73	0.106	45.686
8.38	0.199	85.769
9.9	0.319	137.489



Points in the above graph represent Shinoda data and the curve is simply a "best-fit" of those data.

It is important to note that C-8 in aqueous solution will exist primarily as ions according to the electrolyte dissociation reaction

$$NH_4PFO = NH_4^+ + PFO^-$$

where PFO represents the perfluoro-octanoate portion of the C-8 molecule. This dissociation will affect the volatility of C-8 from aqueous solutions.

Ions are not volatile from aqueous solutions within normal temperature ranges (at temperatures less than the critical point of water). Therefore, if the component in question exists as an ion in solution, the component will still be volatile, but the mole fraction of component able to volatilize will be the mole fraction of the un-dissociated molecular species in solution, not the total concentration. The mole fraction of un-dissociated compound can be calculated from the dissociation constant, and for the general reaction

$$Salt = Cation^{+} + Anion^{-}$$

is expressed as

$$K_i = \frac{[Cation^{+}] * [Anion^{-}]}{[Salt]}$$

K_I is a thermodynamic property which is a function of the components and temperature.

For C-8, $K_I = 4570$, so up to the point of saturation (where a second phase of un-dissociated C-8 exists) only a very small fraction of the C-8 in aqueous solution will be available for volatilization. For example, according to the Shinoda data at 1.58°C, the solubility of C-8 is 0.0339 gmole/liter. At this concentration, only 0.0007% of the C-8 exists in molecular form (NH_4PFO) capable of volatilization.

pH will also have an effect on the existence of C-8 (as the ammonium form of the compound) in aqueous solution. If the pH decreases to levels approximately <2.2, the formation of perfluoro-octanoic acid will occur according to the reaction

$$PFO^{-} + H^{+} = HPFO.$$

This reaction will prevent formation of the ammonium form of the compound by removing PFO^{-} from the C-8 equilibrium reaction. Likewise, if the pH increase to levels approximately >9.2, ammonium ions will de-protonate according to the reaction

$$NH_4^{+} = NH_3 + H^{+}.$$

This reaction will prevent formation of the ammonium form of the compound by removing NH_4^{+} from the C-8 equilibrium reaction.