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ABSTRACT .WATERLESS WATER:

The Faustian Bargain of Physical Chemists and Biologists

A gallimaufry of phenomena in biology and physical chemistry depend on specific ion or Hofmeister effects, inexplicable by classical theories or by simulation. These involve “waterless”, water, and ignore all important effects of dissolved gas responsible for long range hydrophobic interactions.

In the classical theories of electrolytes ion specificity occurs only in “hidden variables”, fitting parameters like ion size. In simulation the model water is unreal as it ignores solutes. The theories are fundamentally flawed. This is so for concepts like pH, buffers , pKas, interactions of ions with surfaces, membrane and zeta potentials, colloidal interactions and ion pumps. Biochemists and biologists use the techniques and the intuition of the physical chemistry. The interpretation of standard measurements depends on the classical theory. So if the theory is incorrect or flawed so is the meaning of the measurement, e.g of a pH, pKa, or a membrane potential.

We have a muddle, a mishmash of unexplained phenomena associated with specific ion effects, water structure and hydration glossed over in a kind of Faustian bargain.

The result is a proliferation of parameters that lack predictability in a Ptolemaic system. Except that the Ptolemaic system worked! Add to the situation the fact that dissolved atmospheric gas strongly affects everything else, like hydrophobic interactions in a way that is itself ion specific; and is ignored in simulation. Then the known knowns , known unknowns and unknown unknowns of Rumsfeld all become unknowns.

Despite this depressing scenario, when recent developments of our understanding of specific ion effects are brought to bear, many of the observations do begin to fall into place.

