THE WATER PAIR POTENTIAL: CONFRONTATION BETWEEN EXPERIMENTS AND THEORY

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The liquid water potential, i.e. the intermolecular forces acting between individual molecules is not yet accurately known. We describe recent attempts which have been made at the elucidation of its primary component : the *pair potential* between two molecules only. Its description relies on the confrontation between spectroscopical experiments on water clusters produced in molecular beams, and exact quantum calculations using as input the simple MCY potential of Clementi and coll. This *rigid* model was first fitted in order to reproduce the observed transitions frequencies in the far Infra-red spectrum.
Internal motions of the monomers (stretches and bends) were then explicitely considered by invoking an adiabatic separation between the slow (intermonomeric) and fast (intramonomeric) modes. This formulation allows one to recast the calculations into an equivalent six-dimensional problem ($\sim$ rigid monomers) on an *adiabatic* potential energy surface. Our model MCY potential was then fitted to a fully flexible pair potential, which leads to very good agreement with all observed frequencies.