GETTING TO THE CORE OF WATER

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In the famous water potential of Partridge and Schwenke (PS) [J.Chem.Phys **106** 4618 (1997)], the critical ingredient for the very successful fit to experimental data was the inclusion of core-valence correlation. Other corrections to the potential, such as scalar relativity and Born-Oppenheimer breakdown, are of non-negligible size,[Polyansky *et al.* Science **299** 539 (2003)] but can be easily modeled empirically. A drawback of the PS calculation of the core-valence correction was it was carried out using just one basis set, and that the quality of the basis set was unknown. We have developed a new method for judging the quality of core-valence basis sets, and this has enabled us to optimize a new hierarchy of basis sets for treating core-valence correlation in a much more systematic manner. These new basis sets will be used to provide a new, more accurate, calculation of the core-valence correction to the potential, dipole moment and spectrum of water.