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MAME Water Model: hydrogen bonding, electrostatic, polarization and van der Waals interactions in water. EUGENE TSIPER — Hydrogen bonding is key to many unusual properties of water and its role in biological systems. I will describe an elegant water model derived using the minimal atomic multipole expansion (MAME). The minimal set for water consists of three multipoles that are chosen to satisfy experimental molecular dipole and both components of the molecular quadrupole. Two atomic polarizabilities, $\alpha_O = 1.4146$ A^3 and $\alpha_{\rm H} = 0.0836$ A^3, reproduce all three components of the polarizability tensor due to a relation between the latter, which follows from the model and is indeed satisfied experimentally. The model thus based on the known monomer properties reproduces hydrogen bonding in the dimer and compares favorably to the best available water-water interaction potentials. I will also discuss the meaning of distributed polarizabilities for computing dispersion (van der Waals) interactions. The atomic polarizabilities in water yield reasonable dispersion energy of 1.4 kcal/mol, which is otherwise underestimated when water molecules are treated as polarizable points. [E.V. Tsiper, Phys. Rev. Lett. 94, 013204, 2005]

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