DIMERIZATION OF WATER MOLECULES. MODELING OF THE ATTRACTIVE PART OF THE INTERPARTICLE POTENTIAL IN THE MULTIPOLE APPROXIMATION

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S u m m a r y

The work presents the detailed analysis of the water dimer properties. Their parameters are investigated on the basis of a multipole interaction potential extended up to the quadrupole–quadrupole and dipole–octupole terms. All main equilibrium parameters of the dimer are obtained: its geometry, ground-state energy, dipole and quadrupole moments, vibration frequencies, *etc.* They are thoroughly compared with those obtained in quantum chemical calculations and from spectroscopic data. The efficiency of the present model potentials is discussed. A new viewpoint on the nature of the hydrogen bond is presented. The results of studies are thoroughly compared with the spectroscopic and computer simulation data.