CALCULATING H_2O STATES UP TO DISSOCIATION STATES USING PDVR3D

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Even small chemically bound molecules have 10^5 or more bound states. Calculations of this size represent a grand challenge to conventional computers. We have parallelized DVR based program suite DVR3D(1) to give PDVR3D(2). The PDVR3D suite runs on the Cray T3D/T3E at Edinburgh University(U.K.), the IBM SP2 at Daresbury(U.K.) and on the Cray T3E at CINECA (Italy).
As a first application of PDVR3D, we are studying the water molecule using two newly available global potentials due to Varandas(3) and Ho and Rabitz(4). We have calculated the ro-vibrational levels of water up to dissociation limits for both potentials. Studies of bound and quasibound ro-vibrational states of H_3^+, using a realistic global potential(5), are also being performed.

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