THEORETICAL INVESTIGATION OF ROVIBRATIONAL SPECTRA OF $(HF)_2$ AND ITS ISOTOPIC SUBSTITUTES — CENTRIFUGAL DISTORTION, TUNNELING SPLITTING

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An efficient parallel algorithm is used to calculate the rovibrational spectrum of the HF dimer and its isotopic substitutes. The algorithm solves the quantum mechanical problem for all six internal degrees of freedom. Tests on a CRAY T3E show that the parallel algorithm scales almost linearly as the number of processors is increased from 1 to 128. Meanwhile, the parallel algorithm reduces the computational time from tens of hours on a workstation to ten minutes or less on a massively parallel supercomputer.

The spectral analysis shows that although the minimum energy geometry of $(HF)_2$ is bent, the system behaves like a quasi-linear molecule due to the large amplitude zero point motions. Many interesting experimental observations on the HF dimer and its isotopic substitutes are explained by a quasi-linear molecule model, including the large centrifugal distortion at low K, the positive correlation between the tunneling splitting and K.