AN IMPROVED *AB INITIO* POTENTIAL ENERGY SURFACE FOR CH_4

D. W. SCHWENKE, *NASA Ames Research Center, Moffett Field, CA 94035-1000*.

The reliable calculation of ro-vibrational energy levels and line strengths requires a good potential energy surface (PES). The best ab initio PES for CH4 does well on bending vibrations, but systematically under predicts the stretching frequencies by several cm^{-1}. In this work, we report our progress in understanding and resolving this dilemma.The two most uncertain parts of the ab initio calculations are the convergence of the one electron basis set, and the convergence of the treatment of electron correlation. These appear to arise because of the importance of the ^5S state of C in the bonding of methane.