MICROWAVE AND HIGH RESOLUTION INFRARED SPECTRA OF VINYL CHLORIDE, AB INITIO ANHARMONIC FORCE FILD AND EQUILIBRIUM STRUCTURE

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The quadratic, cubic and semi-diagonal quartic force field of vinyl chloride has been calculated at the MP2 level of theory employing a basis set of triple-zeta quality. The spectroscopic constants derived from this force field are compared to the experimental values. To make this comparison more complete, the rotational constants of the lowest excited state, v_9= 1 have been determined by microwave spectroscopy and the ν_{12} band has been investigated by high-resolution infrared Fourier transform spectroscopy. The equilibrium structure has been derived from experimental ground state rotational constants and ab initio rovibrational interaction parameters. This semi experimental structure is in excellent agreement with the ab initio structure calculated at the CCSD(T) level of theory using a basis set of quintuple-zeta quality and a core correlation correction. The experimental mass-dependent rm structures are also determined and their accuracy is discussed.