AB INITIO AND INFRARED SPECTROSCOPIC STUDIES OF THE PROPYLENE OXIDE - CARBON DIOXIDE COMPLEX

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High resolution infrared spectroscopy and *ab initio* calculations of chiral molecules and their molecular complexes promise to provide rich structural and dynamical information about this important class of molecular systems. Our present work focuses on the infrared spectroscopic study of the propylene oxide-CO_2 complex in the region of the CO_2 asymmetric stretching vibration. The experiments were carried out using a fast scan mid-infrared lead salt diode laser spectrometer in combination with a pulsed slit expansion. Complete geometry optimization and harmonic vibrational frequency calculations were performed for the propylene oxide-CO_2 complex using the MP2 level of theory with the cc-pVDZ basis set. The experimental spectroscopic parameters will be compared with those from the *ab initio* calculations.