INFRARED ABSORPTION OF GASEOUS c-CLCOOH AND t-CLCOOH RECORDED WITH A STEP-SCAN FOURIER-TRANSFORM SPECTROMETER

YUAN-PERN LEE AND LI-KANG CHU, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.*

Two conformers of ClCOOH were produced upon irradiation at 355 nm of a gaseous flowing mixture of Cl_2, HCOOH, and N_2. A step-scan Fourier-transform infrared spectrometer coupled with a multipass absorption cell was utilized to monitor the transient spectra of ClCOOH. Absorption bands with origins at 1808.0 and 1328.5 cm^{-1} are attributed to the C=O stretching and COH bending modes of t-ClCOOH, respectively; those at 1883.0 and 1284.9 cm^{-1} are assigned as the C=O stretching and COH bending modes of c-ClCOOH, respectively. These observed vibrational wavenumbers agree with corresponding values for t-ClCOOH and c-ClCOOH predicted with B3LYP/aug-cc-pVTZ density-functional theory and the observed rotational contours agree satisfactorily with simulated bands based on predicted rotational parameters. The observed relative intensities indicate that t-ClCOOH is more stable than c-ClCOOH by 3 kJ mol^{-1}. A simple kinetic model is employed to account for the production and decay of ClCOOH.