

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

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Two conformers of ClCOOH were produced upon irradiation at 355 nm of a gaseous flowing mixture of Cl₂, HCOOH, and N₂. 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.