

HIGH RESOLUTION SPECTRA OF THE SIMPLEST CRIEGEE INTERMEDIATE CH₂OO BETWEEN 880 AND 932 cm⁻¹

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The Criegee intermediates (CI) play critical roles in atmospheric chemistry. CH₂OO is the simplest CI and its characterization is important for investigations of reaction mechanisms and molecular structure. In this work, high-resolution spectra of the OO-stretching (ν_6) mode of CH₂OO in the range of 880–932 cm⁻¹ have been recorded using a quantum cascade laser (QCL) system coupled with a multi-pass Herriott cell. The CH₂OO was produced from the reaction of CH₂I + O₂ in a flowing mixture of CH₂I₂/O₂ (1/213) at 3.2 Torr upon irradiation at 248 nm with an excimer laser. The spectrum was recorded by step-scanning the QCL with a step size of 0.0016 cm⁻¹; its wavelength was calibrated with a C₂H₄ reference cell and a germanium etalon. Over one thousand lines were assigned and used for fitting of molecular constants of CH₂OO. Furthermore, the rotational perturbations on the high-J levels of K_a = 3, K_a = 6, and K_a ≥ 11 were observed.