DETECTION OF CLSO WITH TIME-RESOLVED FOURIER-TRANSFORM INFRARED ABSORPTION SPECTROSCOPY

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A step-scan time-resolved Fourier-transform infrared spectrometer operated in absorption mode was employed to detect ClSO, which was produced as a reaction intermediate upon irradiation of a flowing mixture of Cl_2SO and Ar with an excimer laser at 308 nm. In the region 1050-1250 cm^{-1}, a transient absorption band, which diminished at prolonged reaction period, indicates a transition associated with the S-O stretching (ν_1) mode of ClSO. A spectrum at 0.13-cm^{-1} resolution partially reveals rotational structure with the Q-branch peaked at 1163 cm^{-1}. Calculations with density-functional theory (B3LYP/aug-cc-pVTZ) predict the geometry, vibrational and rotational parameters of ClSO. A simulated absorption spectrum based on these parameters agrees satisfactorily with experimental observation.