IR SPECTROSCOPY AT THE CANADIAN LIGHT SOURCE: THE ν_{11} FUNDAMENTAL AND $\nu_{16} + \nu_{18}$ - ν_{18} HOT BAND OF TRANS-ACROLEIN

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The ν_{11} fundamental and the $\nu_{16} + \nu_{18}$ - ν_{18} hot band have been identified in the high-resolution Fourier transform spectrum of trans-acrolein (CH_2=CH-CH=O) recorded in the 10-μm region on the Far-Infrared beamline of the Canadian Light Source synchrotron in Saskatoon. The two bands are centered at 912 cm^{-1} and 957 cm^{-1}, respectively, with the excited ν_{11} state corresponding to the A' in-plane CH_2-rocking mode and the ν_{16} $+ \nu_{18}$ state to the combination of the A'' out-of-plane CH_2 rock with the low-frequency (158 cm^{-1}) A'' C-C torsional mode.This extends our previous work on the ν_{14} and ν_{16} fundamentals centered at 993 and 959 cm^{-1}, leaving only the ν_{15} mode now to be assigned at high resolution in the 10-μm spectral region for this important atmospheric pollutant. The ν_{11} band is type a/b and the $\nu_{16} + \nu_{18}$ - ν_{18} hot band is c-type, so that assignments could be confirmed by lower-state combination differences. The assigned transitions have been fitted to a Watson asymmetric rotor Hamiltonian, and molecular parameters for both states will be reported.