ANALYSIS OF HIGH RESOLUTION INFRARED SPECTRA OF 1,1-DICHLOROETHYLENE IN THE $500 - 1000$ cm^{-1} RANGE

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The far infrared beamline of the Canadian Light Source synchrotron facility has been used to record three rotationally resolved vibrational bands of 1,1-dichloroethylene in the $500 - 1000$ cm^{-1} range, at 0.00096 cm^{-1} resolution. These correspond, for the $H_2C{=}C^{35}Cl_2$ isotopologue, to an a-type band (CCl_2 antisymmetric stretch) at 796.0 cm^{-1}, a b-type band (CCl_2 symmetric stretch) at 603.0 cm^{-1}, and a c-type band (CH_2 wag) at 868.6 cm^{-1}. Anharmonic frequency calculations at the MP2/6-311++G(2d,2p) level, combined with rotational and centrifugal distortion constants from a millimeter wave study of the ground state[a], were an invaluable aid in facilitating the spectroscopic assignment for this asymmetric top ($\kappa = -0.58$). Analysis of the 796 cm^{-1} band is nearly complete, giving well determined excited state rotational and centrifugal distortion constants. Results of this analysis and progress with analysis of the other two bands will be presented.

[a] Z. Kisiel, L. Pszczółkowski, *Z. Naturforsch*, **50a**, (1995), 347-351.