

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 $\text{H}_2\text{C}=\text{C}^{35}\text{Cl}_2$ 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.

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