SYNCHROTRON BASED HIGH RESOLUTION FAR-IR SPECTROSCOPY OF 1,1-DICHLOROETHYLENE

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Six vibrational bands of the $^{35}Cl_2C{=}CH_2$ isotopologue of 1,1-dichloroethylene have been recorded in the 350 – 1150 cm^{-1} range using the 0.00096 cm^{-1} resolution far-infrared beamline of the Canadian Light Source synchrotron facility. Results from the analysis of one a-type (ν_9 = 796.01904(8) cm^{-1}, CCl asymmetric stretch) and one c-type (ν_{11} = 868.488626(26) cm^{-1}, CH_2 flap) band will be presented. Over 6000 transitions have now been fitted for these two bands, with ground state rotational and centrifugal distortion constants fixed to values determined by rotational spectroscopy,[a] while the upper state constants have been varied. Anharmonic frequency calculations at the MP2/6-311++G(2d,2p) level were instrumental in assigning the dense spectra. Assignment of additional bands around 603 cm^{-1} (b-type, CCl symmetric stretch, ν_4) and 456 cm^{-1} (c-type, CCl_2 flap, ν_{12}), as well as attempts at assigning the mixed $^{35}Cl^{37}Cl$ isotopologue spectra for ν_9 and ν_{11}, are in progress.

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