

FIRST HIGH RESOLUTION IR STUDY OF THE ν_{14} (A') A-TYPE BAND NEAR 421.847 cm^{-1} OF $2\text{-}^{13}\text{C}$ -PROPENE

S.J. DAUNT, ROBERT GRZYWACZ, *Department of Physics & Astronomy, The University of Tennessee-Knoxville, Knoxville, TN, USA*; BRANT E. BILLINGHURST, *EFD, Canadian Light Source Inc., Saskatoon, Saskatchewan, Canada*.

This is the first high resolution IR study of any band of the $2\text{-}^{13}\text{C}$ -propene species. There have been only two previous high resolution studies of vibration-rotation bands of the normal species.^a The band examined here is the ν_{14} (A') CCC skeletal bending near 421.847 cm^{-1} which has an A-Type asymmetric rotor structure. The spectra were recorded on the FTS at the Far-IR beamline of the Canadian Light Source with a resolution of $\Delta\nu = 0.0009\text{ cm}^{-1}$. We have assigned and fitted around 2200 transitions and determined ground and upper state rotational constants. Lines with J up to 49 and K up to 12 were included. The subbands with K greater than 12 were perturbed and show torsional splittings that vary from small to extremely large. The fitting was done with the PGOPHER program of Colin Western.^b The GS constants are in good agreement with the MW constants reported recently by Craig, Groner and co-workers.^c

^aAinetschian, Fraser, Ortigoso & Pate, *J. Chem. Phys.* **100**, 729 ff. (1994); Lafferty, Flaud & Herman, *J. Mol. Struct.* **780-781**, 65 ff. (2006).

^bWestern, *J. Quant. Spectrosc. Rad. Transf.* **186**, 221 ff. (2017).

^cPaper M109, 71st ISMS Symposium (2016); *J. Mol. Spectrosc.* **328**, 1-6 (2016).