FIRST HIGH RESOLUTION IR STUDY OF THE ν_{14} (A') A-TYPE BAND NEAR 421.847 cm⁻¹OF 2-¹³C-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 is the first high resolution IR study of any band of the 2-¹³C-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 $\Delta \nu = 0.0009$ 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).