THE MILLIMETER WAVE SPECTRUM OF LINALOOL

COREY J EVANS, STEPHANIE M ALLPRESS, *Department of Chemistry, University of Leicester, Leicester, LE17RH, United Kingdom*; PETER D GODFREY, DON MCNAUGHTON, *School of Chemistry, Monash University, 3800, Victoria, Australia*.

The millimeter wave spectrum (48-72 GHz) of linalool has been recorded for the first time. Over 40 conformers of S-(+) and R-(-)-linalool have been investigated using computational chemistry techniques, with 10 conformers predicted to be within 400 cm^{-1} of the lowest lying isomer at the B3LYP/aug-cc-pVTZ level of theory. The observed lines can be assigned to two conformers of (S)-(+)-linalool. Precise rotational and centrifugal distortion constants have been determined for both conformers.