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THE COMPLETE HEAVY-ATOM STRUCTURE OF A CP-FTMW CHIRAL TAG PRECURSOR, VERBENONE

FRANK E MARSHALL, *Department of Chemistry, Missouri University of Science and Technology, Rolla, MO, USA*; CHANNING WEST, GALEN SEDO, *Department of Natural Sciences, University of Virginia's College at Wise, Wise, VA, USA*; BROOKS PATE, *Department of Chemistry, The University of Virginia, Charlottesville, VA, USA*; G. S. GRUBBS II, *Department of Chemistry, Missouri University of Science and Technology, Rolla, MO, USA*.

The microwave spectrum of the chiral molecule verbenone has been recorded from 2-18 GHz using two CP-FTMW spectrometers. 2-8 GHz data has been acquired on a 2-8 GHz CP-FTMW located at the University of Virginia and 8-18 data has been acquired on a 6-18 GHz spectrometer located at Missouri S&T. From the experiments the authors were able to assign and fit isotopologues corresponding to each heavy atom position (either ^{13}C or ^{18}O), providing for the heavy-atom structure. Previous studies by Evans and coworkers have been added to these measurements in a global fit of the parent species.[a,b] The measurement and assignment of these transitions provide preliminary information needed for enatiomeric excess experiments using CP-FTMW van der Waals-type chiral tagging processes already being performed at UVa. Details of the experiment, fits, and structure will be discussed.

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[a] C. J. Evans, S. M. Allpress, P. D. Godfrey, D. McNaughton, *67th International Symposium on Molecular Spectroscopy*, 2012, **RH13**

[b] S. M. Allpress, *Spectroscopic and Computational Chemistry Studies on Terpene Related Compounds*, University of Leicester, 2015, Chapter 6: Microwave Spectroscopy of Verbenone