POPULATION ENHANCEMENT AND ROTATIONAL CHARACTERIZATION OF GAUCHE-ISOPRENE BY HIGH RESOLUTION FTMW SPECTROSCOPY

JESSIE P PORTERFIELD, Radio and Geoastronomy Division, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA; J. H. WESTERFIELD, Department of Chemistry, The University of California, Davis, CA, USA; LINCOLN SATTERTHWAITE, DAVID PATTERSON, Physics, University of California, Santa Barbara, CA, USA; BRYAN CHANGALA, JILA, National Institute of Standards and Technology and Univ. of Colorado Department of Physics, University of Colorado, Boulder, CO, USA; JOSHUA H BARABAN, Chemistry, Ben-Gurion University of the Negev, Beer-Sheva, Israel; MICHAEL C McCARTHY, Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA.

Isoprene is a highly abundant species in the atmosphere, second only to methane in hydrocarbon emissions. There are two stable conformers of isoprene, trans and gauche, and due to the fact the ground state trans is highly abundant at room temperature (97%), its microwave spectrum has been known since the 1960's. The gauche conformer, however, has evaded microwave observation until now. We have characterized the rotational parameters for the inversion states $(0^+/0^-)$ of gauche-isoprene, aided by high levels of theory and two complementary, high resolution Fourier transform microwave (FTMW) techniques: cavity enhanced FTMW coupled to a pulsed discharge nozzle, and chirped-pulse FTMW in a cryogenic buffer gas cell. Thermal enhancement (from 1.7% up to 10.3%) of the gauche population of isoprene is demonstrated with inlet temperatures ranging from 300-450 K in the cryogenic buffer gas cell. This work demonstrates for the first time that the buffer gas cell is well suited for thermochemical studies similar to matrix isolation spectroscopy, but by far simpler and more rapid analytical means.

