# HIGH-RESOLUTION INFRARED SPECTROSCOPY OF JET-COOLED CYCLOPROPYL RADICAL: IN-PHASE ANTISYMMETRIC $CH_2$ STRETCHING VIBRATIONS

FENG DONG, ERIN S. WHITNEY, and DAVID NESBITT, *JILA, University of Colorado, Boulder, CO 80309*.

The retention or inversion of substituted cyclopropyl radical has been a very interesting issue for decades. Recently, the high-resolution infrared spectra of jet-cooled cyclopropyl radical in the in-phase antisymmetric $CH_2$ stretching region have been obtained in our slit jet discharge spectrometer. Two vibrational bands have been assigned to the lower- to-lower and upper-to-upper vibrational bands, due to the tunneling splitting of the lone CH bending perpendicular to the carbon plane. Most of the transitions are well fit to an asymmetric top Hamiltonian, which provides the band origins and rotational constants for both tunneling levels. The tunneling splitting for the ground and excited states are obtained at $3.4\text{cm}^{-1}$ and $5.1\text{cm}^{-1}$. The barrier for the tunneling has been calculated to be 1.8Kcal/mol at MP2/6-311++G(3df,3pd) level. These results explain why the cyclopropyl radical is a highly reactive inverting radical reported in the kinetic measurements[a].

[a] L.J.Johnston and K.U. Ingold, J. Am. Chem. Soc., 108, 2343 (1986)