RING-OPENING OF CYCLOPROPYL RADICAL TO ALLYL RADICAL

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

The possibilities of the ring-opening of the cyclopropyl radical to allyl radical and the ring-closure of allyl radical to cyclopropyl radical have been a long-standing question in both experimental and theoretical studies. With a barrier of 22.5kcal/mol, it has been predicted that the ring-opening is topologically disrotatory and hence forbidden, but the release of the ring strain should make it easier to lead to the allyl radical. In our recent studies of cyclopropyl radicals produced in a slit jet discharge of Bromocyclopropane, the high-resolution infrared spectra of v2 vibrational band of allyl radical has been observed, which is the product of the ring-opening of cyclopropyl radical. The population ratio of allyl radical is about 10cyclopropyl radical. Possible ring-opening mechanisms will also be discussed.