FIRST HIGH RESOLUTION INFRARED SPECTROSCOPY OF GAS PHASE CYCLOPENTYL RADICAL: STRUCTURAL AND DYNAMICAL INSIGHTS FROM THE LONE CH STRETCH REGION

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There is a steadily growing interest in alternative fuel sources from extensive heavy oil and tar sand basins known to be plentiful in Canada, Venezuela and China. One major difference between these heavy oil deposits and other sources is the high concentration of cycloalkane species, specifically cyclopentanes and cyclohexanes. Chemical transformation pathways for such species are initiated by H atom removal to form highly reactive cycloalkyl radicals, about which little is known spectroscopically. We have quite recently obtained first high resolution spectra of cyclopentyl radical, formed at roughly 15 K in a slit discharge mixture of Ne/He and 0.1-0.2% cyclopentyl iodide, and corresponding to fundamental excitation of the lone CH stretch on the sp^2 hybridized carbon radical center. This band origin occurs near 3071 cm^{-1}, blue shifted considerably from the normal sp^3 hybridized methylenic CH_2 stretch region, which proves helpful in eliminating interference due to precursor absorption. A complete analysis is underway, progress toward which will be reported. Of particular interest in such spectral analysis will be barriers between conformations (e.g., envelope vs twist) and in general the role of pseudorotation dynamics in cyclopentane vs cyclopentyl radical.