

JET-COOLED LIF SPECTRA OF CYCLOHEXOXY RADICALS

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Cyclohexoxy is a key intermediate in the atmospheric oxidation of cyclohexane, which constitutes up to 1% automotive fuel. We recently obtained moderate resolution laser excitation spectra of cyclohexoxy in free jet expansion at temperatures of order 1 K and 100 K. Some of the excitation lines disappear in the colder expansion and this observation along with different rotational contours for various vibronically resolved bands suggest multiple conformers exist in the jet. Ab initio calculations have been performed to predict the geometry, rotational constants and relative energy of the different conformers of cyclohexoxy. Initial spectral assignments will be discussed in this talk. Work is in progress to obtain high resolution rotationally resolved spectra to make unambiguous conformational assignments and characterize their structures.