SYNTHESIS AND MILLIMETER-WAVE SPECTRA OF CYCLOPROPANONE: VIBRATIONAL GROUND STATE AND FOUR VIBRATIONALLY EXCITED STATES

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Cyclopropanone is a fundamental, strained organic compound as the smallest cyclic ketone. It is also a potential astrochemical molecule that has been reported by Abplanalp et al. in 2015 to form on ices consisting of carbon monoxide and ethylene when bombarded by high-energy electrons.[1] Despite this, searches for cyclopropanone in the interstellar medium has been hampered by a lack of available rotational data beyond 40 GHz. Its microwave spectrum has been studied previously by Flygare and coworkers in 1969, who reported 15 transitions and determined its rotational constants.[2] Its rotational spectrum has not been reinvestigated, presumably due to the difficulty of obtaining a pure sample. Recently, we have been able to produce cyclopropanone from ketene and diazomethane in diethyl ether. Herin, we report, the rotational spectra of cyclopropanone from 85-750 GHz and a least-squares fit of its ground state using A- and S-reduction, sextic, centrifugally distorted Hamiltonians. Likewise, we have measured, assigned and least-squares fit transitions for the four lowest energy vibrationally excited states. The two lowest energy fundamentals (ν_{18}, ν_{14}) have been adequately fit to single-state Hamiltonians. The next fundamental (ν_9) and first overtone presented in this work ($2\nu_{18}$) exhibit perturbed frequencies due to Coriolis and anharmonic coupling. The current progress towards satisfactory treatments of these interactions will be presented.

[1]M. K. Abplanalp, A. Borsuk, B. M. Jones, R. I. Kaiser, Apj. 2015, 814, 45. [2]J. M. Pochan, J. E. Baldwin, W. H. Flygare, J. Am. Chem. Soc. 1969, 91, 8, 1896-1898