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Temperature Dependent Raman Intensities and Calculations of Chiral ketone Conformers WATHEQ AL-BASHEER, The Hashemite University, Zarqa 13115, JUN LI, Pacific Northwest National Laboratory, Richland, WA 99352, ROBERT COMPTON, The University of Tennessee, Knoxville, TN 37996 — Vibrational Raman spectra for the C-H stretch region of *R*-(+)-3-methylcyclopentanone (*R*3MCP) neat sample as a function of temperature variation will be presented and employed as a conformational analysis method. Probing the methyl group C-H stretch region (2850 – 3000 cm^{-1}) relative peak intensities of assigned conformers, is being manipulated to determine the conformer energy differences between equatorial methyl and axial methyl isomers. Raman spectroscopy performed under liquid nitrogen (RUN) will also be presented as a preliminary tool to observe Raman vibrational modes at liquid nitrogen temperatures ($\sim$ 77 °K), and to improve resolution and high signal to noise ratio. An observed few wavenumbers bathochromic (red) shift in Raman lines frequencies will be attributed to sample phase change. The validity of Density Functional Theory (DFT) calculations, of different levels basis sets, for *R*3MCP conformers Raman intensities and frequencies will be investigated and compared against experimental findings.

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