FTIR OF METHYL PYRUVATE CONFORMERS IN AN ARGON MATRIX

ALLISON B. COMBS, JORDAN L. PRESTON, SARA E. LILLY, COURTNEY D. HATTEN, and LAURA R. MCCUNN, Department of Chemistry, One John Marshall Drive, Huntington, WV 25755.

Methyl pyruvate has been isolated in a low-temperature argon matrix and its vibrational spectrum recorded by FTIR. The spectrum is compared to results from B3LYP/6-311++G** optimization and frequency calculations for the s-cis and s-trans conformers of methyl pyruvate. The s-cis conformer of methyl pyruvate is predicted to have an energy of 1.03 kcal/mol relative to the s-trans conformer, with a barrier height of 2.66 kcal/mol for interconversion between the two conformers. Unique bands of both conformers have been identified in the FTIR spectrum and then compared to the simulated spectra to determine that matrix-isolated methyl pyruvate is composed of approximately 92% s-trans conformer.