FTIR OF METHYL PYRUVATE CONFORMERS IN AN ARGON MATRIX

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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.