

Abstract Submitted
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Raman Spectra and the Potential Energy Function for the Internal Rotation of 1,3-Butadiene and its Isotopomers¹ JAAN LAANE, PRAVEENKUMAR BOOPALACHANDRAN, Texas A&M University, NORMAN CRAIG, Oberlin College — The gas-phase Raman spectra of 1,3-butadiene-d₀, 2,3-d₂, 1,1,4,4-d₄, and -d₆ have been collected with CCD detection with numerous scans of ten hours or more. For each isotopomer eight Raman transitions in the 240-330 cm⁻¹ region corresponding to double quantum jumps of the A_u internal rotation (ν_{13}) were observed for the *trans* conformer. Weaker bands in the 170-260 cm⁻¹ region were assigned to the *gauche* conformation, which lies at higher electronic energy. A periodic potential function for the internal rotation, which fits the data for all the isotopomers, was determined. This function shows the *gauche* form to be 966 cm⁻¹ higher in energy and the barrier between the *trans* and *gauche* structures to be 2055 cm⁻¹. The *cis* structure has an energy 408 cm⁻¹ higher than the *gauche*. Fourteen combination band or hot band series involving ν_{13} for the *trans* conformer were also observed, and these allow the internal rotation levels in various excited vibrational states to be determined.

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