

TOWARD A COMPLETE EQUILIBRIUM STRUCTURE OF BUTADIENE; HIGH-RESOLUTION INFRARED SPECTROSCOPY OF BUTADIENE-1-¹³C₁

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Considerable progress has been made toward obtaining ground state rotational constants for butadiene (BDE) and its isotopomers for use in fitting an equilibrium structure. With the exception of a microwave investigation of the weakly polar BDE-1,1-*d*₂,^a studies of all of the other, nonpolar species have been done with high-resolution (0.002 cm⁻¹) infrared spectroscopy. Rotational constants are available for BDE and BDE-2,3-*d*₂ from one study^b and for the three species of BDE-1,4-*d*₂ from another study.^c The present report is on BDE-1-¹³C₁. The rotational structure in the C-type bands at 524 cm⁻¹, 900 cm⁻¹, and 908 cm⁻¹ in the infrared spectrum has been analyzed. Rotational constants fit to 2191 ground state combination differences derived from all three bands are (in cm⁻¹) *A* = 1.3887919 (6), *B* = 0.1436683 (3), and *C* = 0.1302251 (3). In the parent molecule of *C*_{2h} symmetry, a Raman-active *b_g* mode occurs at 908 cm⁻¹ and an infrared-active mode occurs at essentially the same frequency. In BDE-1-¹³C₁ of reduced, *C_s* symmetry, both modes have significant infrared intensity and occur at 908 and 900 cm⁻¹. The higher frequency mode is CH₂ flapping; the lower frequency one is ¹³CH₂ flapping.^d

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