TOWARD A COMPLETE EQUILIBRIUM STRUCTURE OF BUTADIENE; HIGH-RESOLUTION INFRARED SPECTROSCOPY OF BUTADIENE-1-\textsuperscript{13}C\textsubscript{1}

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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-\textsuperscript{2}D\textsubscript{2},\textsuperscript{a} studies of all of the other, nonpolar species have been done with high-resolution (0.002 cm\textsuperscript{-1}) infrared spectroscopy. Rotational constants are available for BDE and BDE-2,3-\textsuperscript{2}D\textsubscript{2} from one study\textsuperscript{b} and for the three species of BDE-1,4-\textsuperscript{2}D\textsubscript{2} from another study.\textsuperscript{c} The present report is on BDE-1-\textsuperscript{13}C\textsubscript{1}. The rotational structure in the C-type bands at 524 cm\textsuperscript{-1}, 900 cm\textsuperscript{-1}, and 908 cm\textsuperscript{-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\textsuperscript{-1}) $A = 1.3887919 (6)$, $B = 0.1436683 (3)$, and $C = 0.1302251 (3)$. In the parent molecule of $C\textsubscript{bh}$ symmetry, a Raman-active $b\textsubscript{2}$ mode occurs at 908 cm\textsuperscript{-1} and an infrared-active mode occurs at essentially the same frequency. In BDE-1-\textsuperscript{13}C\textsubscript{1} of reduced, $C\textsubscript{a}$ symmetry, both modes have significant infrared intensity and occur at 908 and 900 cm\textsuperscript{-1}. The higher frequency mode is CH\textsubscript{2} flapping; the lower frequency one is $^{13}$CH\textsubscript{2} flapping.\textsuperscript{d}

\textsuperscript{b} N. C. Craig, J. L. Davis, K. A. Hanson, M. C. Moore, and M. Lock J. Mol. Struct. 00, 000, (2004).
\textsuperscript{c} N. C. Craig, K. A. Hanson, R. W. Pierce, S. D. Saylor, and R. L. Sams J. Mol. Spectrosc., submitted.