TOWARD A COMPLETE EQUILIBRIUM STRUCTURE OF BUTADIENE; HIGH-RESOLUTION INFRARED SPECTROSCOPY OF BUTADIENE-1-$^{13}C_1$

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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-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-$^{13}C_1$. 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-$^{13}C_1$ of reduced, C_s symmetry, both modes have significant infrared intensity and occur at 908 and 900 cm^{-1}. The higher frequency mode is CH_2 flapping; the lower frequency one is $^{13}CH_2$ flapping. [d]

[a] W. Caminati, G. Grassi, and A. Bauder *Chem. Phys. Letters* **148**, 13, (1988).
[b] N. C. Craig, J. L. Davis, K. A. Hanson, M. C. Moore, and M. Lock *J. Mol. Struct.* **00**, 000, (2004).
[c] N. C. Craig, K. A. Hanson, R. W. Pierce, S. D. Saylor, and R. L. Sams *J. Mol. Spectrosc.*, submitted.
[d] P. Huber-Wälchli and Hs. H. Günthard *Spectrochim. Acta*, **37A**, 285, (1981); Yu. N. Panchenko, private communication.