TOWARD A COMPLETE STRUCTURE OF BUTADIENE WITH HIGH-RESOLUTION INFRARED SPECTROSCOPY

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Although the structure of butadiene is used in initial discussions of delocalized π-bonding in every organic textbook, the structure of this fundamental molecule is incompletely known. Information about the CCCC backbone comes from electron diffraction studies.[1] Caminati et al have proposed a partial structure from this data, a low-resolution infrared investigation of butadiene,[2] and their MW investigation of butadiene-1,1-d_2.[3] We have begun a high-resolution (0.002 cm^{-1}) infrared investigation of the complete structure of this nonpolar molecule, which is MW-silent. For the normal species, a C-type band due to out-of-plane CH flapping at 908.072 cm^{-1} and a perturbed A-type band due to antisymmetric C=C stretching at 1596.446 cm^{-1} have been analyzed. The ground state rotational constants are A = 1.3903839(10), B = 0.1478862(2), and C = 0.1336942(2) cm^{-1} for a Watson-type Hamiltonian. For the 2,3-d_2 species, the C-type band at 908.044 cm^{-1} has been analyzed to give A = 1.0203626(5), B = 0.1472767(3), and C = 0.1287171(3) cm^{-1} for the ground state rotational constants. Structural implications of these data will be discussed. Currently, we are attempting a stereospecific synthesis of the two 1,4-d_2 isotopomers and have hopes of obtaining the two singly-substituted ^{13}C isotopomers.

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(2) Cole, A. R. H.; Mohay, G. M.; Osborne, G. A. *Spectrochim. Acta* **1967**, 23A, 909.
(3) Caminati, W.; Grassi, G; Bauder, A. *Chem. Phys. Letters* **1988**, 148, 13.