

ROTATIONAL CONSTANTS FOR THE HIGH ENERGY ROTAMER OF 1,3-BUTADIENE

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A region of the IR spectrum of 1,3-butadiene containing only a band of the *s-gauche* rotamer was predicted by quantum mechanical calculations. Investigation of the IR spectrum using Fourier transform spectroscopy in the gas phase revealed the presence of a band at $749.22(20)\text{ cm}^{-1}$ possessing the typical *b*-type contour consistent with the predicted *A* species, (C_2 symmetry) for the ν_{12} band (=CH₂ twist) of the *s-gauche* rotamer. Rotational analysis of this band on the spectrum recorded for the first time at a resolution of 0.64 cm^{-1} yielded $(A' - \tilde{B}') = 0.4455(25)\text{ cm}^{-1}$ and $(A'' - \tilde{B}'') = 0.4478(27)\text{ cm}^{-1}$ ^a. The extremely complicated character of the high resolution spectrum of this band suggests also non-planar *s-gauche* structure.

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