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) cm^{-1} possessing the typical b-type contour consistent with the predicted A species, (C_2 symmetry) for the ν_{12} band (=CH_2 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) cm^{-1} and $(A'' - \tilde{B}'')$ = 0.4478 (27) cm^{-1} [a]. The extremely complicated character of the high resolution spectrum of this band suggests also non-planar *s-gauche* structure.

[a] G. R. De Maré, Yu. N. Panchenko and J. Vander Auwera, *to be published*.