

STRUCTURE AND TUNNELING DYNAMICS OF *gauche*-1,3-BUTADIENE

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We have recently shown that *gauche*-1,3-butadiene is unambiguously non-planar, with a C=C–C=C dihedral angle of about 34°, and readily tunnels between two equivalent *gauche* structures.^a In this talk, subsequent microwave studies of *gauche*-1,3-butadiene and its isotopologues as well as the empirical equilibrium structure will be summarized. The experiments have utilized the complementary techniques of cavity enhanced Fourier transform microwave (FTMW) spectroscopy with a supersonic expansion and chirped-pulse FTMW in a cryogenic buffer gas cell. The structural characterization is complicated by the effects of facile tunneling, and full dimensional *ab initio* rotational-VMP2 calculations have been performed to address this issue. We will show how the tunneling splitting frequency, which ranges between about 0.5 and 2.0 cm⁻¹ (depending on the isotopologue), can be extracted from the experimental spectra by careful examination of tunneling-rotation perturbations.

^aM.-A. Martin-Drumel *et al.*, ISMS 2016, M111