

HIGH-RESOLUTION MID-IR SPECTROSCOPY OF (E)- AND (Z)-1,3-PENTADIENE USING A QUANTUM CASCADE LASER

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Small conjugated dienes serve as one of the prototypical reactants in the Diels-Alder cyclization reaction commonly used in organic chemistry. These dienes exhibit an interesting conformational landscape where the lowest energy conformer is a *trans* conformation with a *gauche* conformer lying 10-15 kJ/mol higher in energy. The *gauche* conformer has only recently been unambiguously identified as a non-planar structure in 1,3-butadiene (the simplest diene) by microwave spectroscopy.[1] We are interested in understanding the effect of the addition of functional groups on the conformational energy landscape of dienes. 1,3-pentadiene presents one of the simplest substitutions with the addition of a methyl group at the end of the 1,3-butadiene unit.

We have measured room temperature high-resolution infrared spectra of both (E)- and (Z)-1,3-pentadiene using an external cavity quantum cascade laser (EC-QCL) in the range of 970-1010 cm^{-1} . These measurements represent the first high-resolution infrared spectra of these molecules reported to date, with individual rovibrational features exhibiting the Doppler-broadened linewidth of about 0.0016 cm^{-1} . Both (E)- and (Z)-pentadiene exhibit a strong C-type rovibrational band (due to a C-H wagging motion) in this region with a strong Q-branch. We will present our analysis of the rotational structure we have observed, which will provide experimental data to verify computational chemistry of these molecules.

[1] J.H. Baraban, M.-A. Martin-Drumel, et al., *Angewandte Chemie*, **57**, 1821 (2018)