

## Accepted Manuscript

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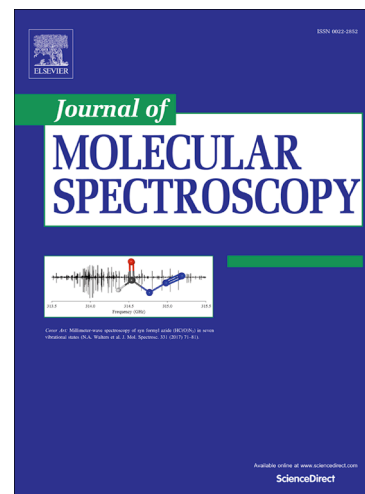
PII: S0022-2852(18)30276-5  
DOI: <https://doi.org/10.1016/j.jms.2018.09.007>  
Reference: YJMSP 11082

To appear in: *Journal of Molecular Spectroscopy*

Received Date: 24 August 2018  
Revised Date: 25 September 2018  
Accepted Date: 26 September 2018

Please cite this article as: G.T. Pullen, P.R. Franke, Y-P. Lee, G.E. Douberly, Infrared Spectroscopy of Propene in Solid para-Hydrogen and Helium Droplets: The Role of Matrix Shifts in the Analysis of Anharmonic Resonances, *Journal of Molecular Spectroscopy* (2018), doi: <https://doi.org/10.1016/j.jms.2018.09.007>

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# *Infrared Spectroscopy of Propene in Solid para-Hydrogen and Helium Droplets: the Role of Matrix Shifts in the Analysis of Anharmonic Resonances*

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## **Abstract**

The infrared spectrum of propene in the CH stretching region is complicated by anharmonic resonance polyads associated with the coupling of CH stretch fundamentals to overtones and combinations of CH<sub>n</sub> bends and CC stretches. We report the spectra of propene isolated in both helium nanodroplets (HENDI) and solid *para*-hydrogen (*p*-H<sub>2</sub>). Spectral assignments and anharmonic polyad memberships are obtained with a VPT2+K effective Hamiltonian. In the 2800 to 3120 cm<sup>-1</sup> region, the average differential matrix shift in going from HENDI to *p*-H<sub>2</sub> is ~4.4 cm<sup>-1</sup> to the red, with a standard deviation of 1.9 cm<sup>-1</sup>. Moreover, the choice of matrix environment influences the positions and intensity ratios of transitions within the resonance polyads. Two-state interaction models are used to confirm that differential matrix shifts less than 10 cm<sup>-1</sup> are sufficient to account for the observed differences.

## **Keywords**

*para*-Hydrogen matrix isolation, Helium nanodroplet isolation, Propene infrared spectroscopy, Anharmonic resonance polyads, Effective Hamiltonian calculations

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