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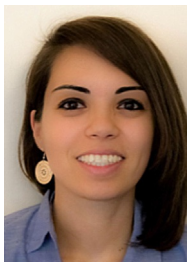
Conformational Flexibility of Limonene Oxide Studied By Microwave Spectroscopy


D. Loru


M.M. Quesada Moreno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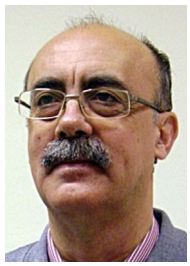
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The front cover artwork is provided by the groups of Prof. J.J. López-González (University of Jaen, Spain), Prof. T.R. Huet (University of Lille, France), and Dr. M.E. Sanz (King's College London, UK). The image shows the five lower-energy conformers of limonene oxide, a molecule of atmospheric interest, identified by microwave spectroscopy. Read the full text of the article at 10.1002/cphc.201600991.

What is the most significant result of this study?

Being able to characterize five conformers of atmospherically-relevant limonene oxide by microwave spectroscopy, including an axial conformer. This work advances spectroscopic studies on monoterpenes and their oxidation and degradation products.

What aspects of this project do you find most exciting?

Linking high-resolution spectroscopy with high-level quantum chemical calculations to atmospheric applications like the characterization of monoterpenoids, which are biogenic volatile organic compounds (BVOCs) that play a major role in atmospheric chemistry by participating in the formation of aerosols.

What was the inspiration for this cover design?

The image summarizes the five identified conformers of limonene oxide and shows the relevance of terpenes (such as limonene, and their oxidation products) in atmospheric chemistry.

Did serendipity play a part in this work?

Detecting for the first time an axial conformer in the gas phase of a monoterpene of atmospheric interest is an unexpected result. The observation of an axial conformer with abundance similar to that of some equatorial conformers challenges assumptions that equatorial forms are generally more stable in cyclic monoterpenoid compounds, and reflects the delicate balance of forces at play in limonene oxide, which include attractive interactions involving the epoxide ring, dispersive interactions involving the isoproprenyl group, and steric effects.

Acknowledgments

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