

THE GIGAHERTZ AND TERAHERTZ SPECTRUM of MONO-DEUTERATED OXIRANE (c-C₂H₃DO)

SIEGHARD ALBERT, ZIQIU CHEN, KAREN KEPPLER, *Laboratory of Physical Chemistry, ETH Zurich, Zürich, Switzerland*; PHILIPPE LERCH, *Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland*; MARTIN QUACK, *Laboratory of Physical Chemistry, ETH Zurich, Zürich, Switzerland*; VOLKER SCHURIG, *Institute of Organic Chemistry, University of Tübingen, Tübingen, Germany*; OLIVER TRAPP, *Department of Chemistry, Ludwig Maximilians University, Munich, Germany*.

The rotational spectrum of the chiral mono-deuterated oxirane c-C₂H₃DO, an isotopomer of oxirane (ethylenoxide), of which the normal isotopomer has already been detected in interstellar clouds, was measured in the ranges 78 to 108 GHz and 25 to 70 cm⁻¹. Thus one can expect that c-C₂H₃DO will be detectable in space in the future given the current accurate laboratory data. c-C₂H₃DO is also of interest as a simple prototypical molecule for isotopic chirality and parity violation.^{a,b,c,d} The Zurich GHz spectrometer and a high resolution FTIR interferometer using synchrotron radiation was used for the THz spectrum.^{d,e,f} Previous laboratory work on the rotational spectrum of deuterated oxirane extended only to the frequency of 45 GHz. A total of 119 transitions have been newly assigned in the GHz range (extended to 119 GHz) up to J=18 and 900 transitions in the THz region at most to J=70. The analyses of the rotational spectra shall be discussed in detail in relation to their astrophysical importance.

^aM. Quack, *Angew. Chem. Int. Ed.* **28**, 571-586 (1989).

^bM. Quack, *Fundamental Symmetries and Symmetry Violations from High-resolution Spectroscopy, Handbook of High Resolution Spectroscopy*, M. Quack and F. Merkt eds., John Wiley & Sons Ltd, Chichester, New York, 2001, vol. 1, ch. 18, pp. 659-722.

^cR. Berger, G. Laubender, M. Quack, A. Sieben, J. Stohner and M. Willeke, *Angew. Chem. Int. Ed.* **44**, 3623-3626 (2005).

^dS. Albert, I. Bolotova, Z. Chen, C. Fábri, L. Horný, M. Quack, G. Seyfang and D. Zindel, *Phys.Chem.Chem.Phys.* **18**, 21976-21993 (2016).

^eS. Albert, I. Bolotova, Z. Chen, C. Fábri, L. Horný, M. Quack, G. Seyfang and D. Zindel, Proceedings of the 20th Symposium on Atomic, Cluster and Surface Physics (SASP 2016), Innsbruck University Press, 2016, pp. 127-130, ISBN:978-3-903122-04-8. and to be published.

^fS. Albert, F. Arn, I. Bolotova, Z. Chen, C. Fábri, G. Grassi, Ph. Lerch, M. Quack, G. Seyfang, A. Wokaun and D. Zindel, *J.Phys.Chem.Lett.* **7**, 3847-3853 (2016).