

## HIGH RESOLUTION INFRARED SPECTROSCOPY OF CYANO-OXIRANE (c-C<sub>2</sub>H<sub>3</sub>OCN)

SIEGHARD ALBERT, *Physical Chemistry, ETH Zurich, Zurich, Switzerland*; ZIQU CHEN, *College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou, Gansu, China*; KAREN KEPPLER, *Physical Chemistry, ETH Zurich, Zurich, Switzerland*; PHILIPPE LERCH, *Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland*; CARINE MANCA TANNER, MARTIN QUACK, *Physical Chemistry, ETH Zurich, Zurich, Switzerland*; JÜRGEN STÖHNER, *ICBT Institute for Chemistry and Biotechnology, ZHAW Zurich University for Applied Sciences, Wädenswil, Switzerland*.

Oxiranecarbonitrile (cyano-oxirane, c-C<sub>2</sub>H<sub>3</sub>OCN) is of interest as a possible chiral precursor molecule of evolution<sup>a</sup>. We have calculated parity violation in this molecule in view of possible experiments and biomolecular homochirality<sup>b</sup>. Its spectrum has been investigated in the millimeter, submillimeter<sup>c</sup> and terahertz<sup>d</sup> regions. We have recorded its infrared spectrum at 295K with resolution 0.0011 cm<sup>-1</sup> using the Zurich Prototype ZP 2001 FTIR spectrometer<sup>e</sup>. We report here the results of the rovibrational analysis transitions associated with the  $\nu_{12}$  (915.3 cm<sup>-1</sup>) and  $\nu_{13}$  (848.2 cm<sup>-1</sup>) fundamentals using a Watson Hamiltonian and the WANG program<sup>f</sup>, including molecular parameters and ground state energies from our work in the THz region<sup>d</sup>. Simulations performed using the parameters reproduce the observed spectrum well. The results are discussed in relation to astrophysical spectroscopic searches and the evolution of biomolecular homochirality<sup>g</sup>.

<sup>a</sup>M. Bolli, R. Micura, A. Eschenmoser, *Chem. Biol.*, **1997**, 4, 309 (and refs. cited therein).

<sup>b</sup>R. Berger, M. Quack, G. Tschumper, *Helv. Chim. Acta.*, **2000**, 83, 1919; M. Quack, *Chem. Phys. Lett.* **1986**, 132, 147; M. Quack, *Angew. Chem. Intl. Ed.*, **2002**, 41, 4618.

<sup>c</sup>M. Behnke, I. Medvedev, M. Winnewisser, F. C. De Lucia, and E. Herbst, *ApJ. Supplement Series*, **2004**, 152, 97.

<sup>d</sup>S. Albert, Ph. Lerch, K. Keppler and M. Quack, *Proceedings of the XX. Symposium on Atomic, Cluster and Surface Physics 2016, (SASP 2016)*, Innsbruck University Press (2016), pp. 165-168 (and refs. cited therein).

<sup>e</sup>S. Albert, K. Albert and M. Quack, *Trends in Optics and Photonics*, **2003**, 84, 177; "Handbook," Vol. 2, pp. 965-1019 (see also f).

<sup>f</sup>D. Luckhaus and M. Quack, *Mol. Phys.*, **1989**, 68, 745; S. Albert, K. Keppler Albert, H. Hollenstein, C. Manca Tanner, M. Quack in "Handbook of High-Resolution Spectroscopy," M. Quack and F. Merkt, Eds., 2011, Vol. 1, Chapter 3, pp. 117-173, Wiley, Chichester.

<sup>g</sup>M. Quack, *Adv. Chem. Phys.*, **2014**, 157, 249 (and refs. cited therein); M. Quack and G. Seyfang, in "Molecular Spectroscopy and Quantum Dynamics," R. Marquardt and M. Quack, Eds., 2020, Ch. 7, pp. 231-282, Elsevier, Amsterdam, see also [www.ir.ETHz.CH](http://www.ir.ETHz.CH)