ANALYSIS OF THE INFRARED SPECTRUM OF ISOTOPICALLY CHIRAL *TRANS*-2,3-DIDEUTEROOXIRANE

S. ALBERT, K. KEPPLER, G. WICHMANN, M. QUACK, *Department of Chemistry and Applied Biosciences, ETH Zurich, 8093 Zurich, Switzerland*; **Z. CHEN**, *College of Chemistry and Chemical Engineering, Lanzhou University, 730000 Lanzhou China*; **J. STOHNER**, *ICBC, ZHAW, 8820 Wädenswil Switzerland*; **V. SCHURIG**, *Institut für Organische Chemie, Universität Tübingen, 72074 Tübingen, Germany*; **O. TRAPP**, *Department of Chemistry, LMU, 80539 München, Germany*

The concept of isotopic chirality is of fundamental interest because it introduces a completely new isotope effect arising from the parity violating weak nuclear force[1,2,3]. It also has possible astrophysical applications. Oxirane (c-C_2H_4O), detected by astrophysical spectroscopy[4], has two isotopically chiral isotopomers, c-C_2H_3DO and *trans*-2,3-dideuterooxirane (c-CHD-CHDO). We have previously reported the analysis of high resolution GHz and THz spectra of c-C_2H_3DO in the context of a possible first astrophysical observation of an isotopically chiral species[5,6]. Following this work, Müller et al. have reported[7] a tentative detection of c-C_2H_3DO and the achiral c-CD_2CH_2O. There have also been ab initio calculations[8] on c-C_2H_3DO and c-C_2H_4O. We have previously reported[9] high resolution GHz and THz spectra of *trans*-c-CHD-CHDO. Here we report results of the analysis of the infrared spectrum of *trans*-2,3-dideuterooxirane, recorded with a resolution of 0.0015 cm^{-1} using the Bruker IFS 125 HR Zürich Prototype (ZP 2001) Fourier Transform spectrometer. We have used the ground state molecular parameters obtained from our analysis[9] and have carried out the rovibrational analysis using Watson's A reduced effective Hamiltonian. The results will be discussed as they pertain to isotopic chirality and molecular parity violation.

[1] M. Quack, *Angew. Chem. Int. Ed.* 1989, **28**, 571.

[2] R. Berger, G. Laubender, M. Quack, A. Sieben, J. Stohner, M. Willeke, *Angew. Chem. Int. Ed.* 2005, **44**, 3623.

[3] M. Hippler, E. Miloglyadov, M. Quack and G. Seyfang, in Handbook of High-resolution Spectroscopy Vol. 2, p. 1069, M. Quack and F. Merkt, Eds., Wiley, Chicester, 2011. See also the recent review by M. Quack, G. Seyfang, G. Wichmann, *Chem. Sci.* 2022, **13**, 10598.

[4] J. E. Dickens, W. M. Irvine, M. Ohishi, M. Ikeda, S. Ishikawa, A. Nummelin, A. Hjalmarson, *ApJ* 1997, **489**, 753.

[5] S.Albert,Z.Chen,K.Keppler,P.Lerch,M.Quack,V.Schurig,O.Trapp, *PCCP* 2019,**21**,3669.

[6] S.Albert,Z.Chen,K.Keppler,M.Quack,J.Stohner,V.Schurig,O.Trapp, 2023 [in prep.].

[7] H. S. P. Müller, J. K. Jørgensen, J.-C. Guillemin, F. Lewen, S. Schlemmer, *J. Mol. Spectrosc.*, 2023, **394**, 111777; *Monthly Notices of the Royal Astronomical Society* 2023, **518(1)**, 185.

[8] C. Puzzarini, M. Biczysko, J. Bloino, and V. Barone, *ApJ* 2014, **785**, 107.

[9] Z. Chen, S. Albert, K. Keppler, M. Quack, V. Schurig, O. Trapp, ISMS 2021, WJ01.