

HIGH-RESOLUTION GIGAHERTZ AND TERAHERTZ SPECTROSCOPY OF THE ISOTOPICALLY CHIRAL MOLECULE TRANS-2,3-DIDEUTERO-OXIRANE(c-CHD-CHDO)

ZIQU CHEN, *College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou, Gansu, China*; SIEGHARD ALBERT, KAREN KEPPLER, 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*.

We report the observation and assignment of the rotational spectra of the isotopically chiral molecule, trans-2,3-dideutero-oxirane (c-CHD-CHDO) measured in the Gigahertz range of 62-110 GHz and in the Terahertz range, 25-80 cm^{-1} (instrumental resolution of 0.00052 cm^{-1}). Normal oxirane (c-C₂H₄O) has been detected by astrophysical spectroscopy in space.^a A small number of lines of trans-2,3-dideutero-oxirane had been previously analyzed in the microwave region^b up to 70 GHz. We have recently^c measured and successfully analyzed the rotational spectrum of monodeutero-oxirane between 65 and 119 GHz using our GHz spectrometer^d, and in the 0.75 to 2.5 THz range measured with our FTIR setup^e at the Swiss Light Source. In the current work, we were able to assign and analyze more than 2500 rotational transitions of the vibronic ground state of trans-2,3-dideutero-oxirane up to J=65. The molecule is also of interest in the context of molecular parity violation, similar to the related molecule fluoro-oxirane^f. Our results are important in relation to isotopic chirality and parity violation^g, and to the possible astrophysical observation of this molecule.

^aJ. E. Dickens, et al., *ApJ*, **1997**, 489, 753; M. Ikeda, et al., *ApJ*, **2001**, 560, 792; J. M. Lykke, et al., *A&A*, **2017**, 597, A53.

^bC. Hirose, *Bull. Chem. Soc. Jap.*, **1974**, 47, 1311.

^cS. Albert, Z. Chen, K. Keppler, Ph. Lerch, M. Quack, V. Schurig, O. Trapp, *Phys.Chem.Chem.Phys.*, **2019**, 21, 3669

^dM. Suter, M. Quack, *Appl. Opt.*, **2015**, 54 (14), 4417; S. Albert, Z. Chen, C. Fabri, Ph. Lerch, R. Prentner, M. Quack, *Mol. Phys.*, **2016**, 114, 2751.

^eS. Albert, Ph. Lerch, M. Quack, *ChemPhysChem*, **2013**, 14, 3204; S. Albert, K. K. Albert, Ph. Lerch, M. Quack, *Faraday Discuss.*, **2011**, 150, 71.

^fH. Hollenstein, D. Luckhaus, J. Pochert, M. Quack, G. Seyfang, *Angew. Chemie*, **1997**, 109 (1,2), 136; R. Berger, M. Quack, J. Stohner, *Angew. Chem. Intl. Ed.*, **2001**, 40, 1667.

^gM. Quack, *Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy*, in *Handbook of High-resolution Spectroscopy*, M. Quack and F. Merkt eds., Vol.1, pp. 659-722 Wiley, Chichester **2011**