Analysis of the Infrared Spectrum of *trans*-*c*-2,3-di-deutero-oxirane and further isotopomers

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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 [1−3]. It also has possible astrophysical applications. Oxirane (ethylene oxide *c*-C_2H_4O), detected by astrophysical spectroscopy in Sgr B2N [4], has two isotopically chiral isotopomers, monodeuterooxirane (*c*-C_2H_3DO) and *trans*-*c*-2,3-dideuterooxirane (*c*-CHD-CHDO). We have previously reported the analysis of high resolution GHz and THz spectra of monodeuterooxirane in the context of a possible first astrophysical observation of an isotopically chiral species [5, 6]. Following this work, Müller et al have reported a tentative detection of *c*-C_2H_3DO and the achiral *c*-CD_2CH_2O toward IRAS 16293-2422B [7]. There have also been ab initio calculations on the spectra of monodeuterooxirane and oxirane [8]. We have previously reported high resolution GHz and THz spectra of *trans*-*c*-CHD-CHDO [9]. Here we report new results of the detailed analysis of the infrared spectrum of *trans*-*c*-2,3-dideuterooxirane (*c*-CHD-CHDO), which we have recorded up to 3600 cm^{-1} with a resolution of 0.0015 cm^{-1} using the Bruker IFS 125 HR Zürich Prototype (ZP 2001) Fourier Transform spectrometer. The instrumental bandwidth is significantly less than the Doppler width of the compound in this region at room temperature. We have used the molecular parameters obtained from our analysis [9] of the ground state of *trans*-*c*-2,3-dideuterooxirane (*c*-CHD-CHDO) and have carried out the rovibrational analysis of regions of interest in the infrared spectrum using Watson's A reduced effective hamiltonian in the I^r representation, including up to sextic centrifugal distortion constants. The results will be discussed as they pertain to isotopic chirality and molecular parity violation.

[1] M. Quack, *Angew. Chem. Int. Ed.*, 1989, **101**, 588.
[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, "Mass and Isotope Selective Infrared Spectroscopy," 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. Science* 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 and O.Trapp, *PCCP,* 2019, **21**, 3669.
[6] S.Albert, Z.Chen, K.Keppler, M.Quack, J.Stohner, V.Schurig and O.Trapp, 2023 [in preparation].
[7] H.S.P. Müller, J.K. Jørgensen, J.-C. Guillemin, F. Lewen, S. Schlemmer,*J. Mol. Spectrosc.,* 2023, **394**, 111777; H.S.P. Müller, J.K. Jørgensen, J.-C. Guillemin, F. Lewen, S. Schlemmer, *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, and O. Trapp, Proc. ISMS 2021, WJ01, 182 (2021).