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

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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[1,2,3]. 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.

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