THE ROTATIONAL SPECTRUM OF $D_2{}^{17}O$: ACCURATE SPECTROSCOPIC AND HYPERFINE PARAMETERS

CRISTINA PUZZARINI, GABRIELE CAZZOLI, *Dipartimento di Chimica "G. Ciamician", Università di Bologna, I-40126 Bologna, Italy*; JUANA VÁZQUEZ, *Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, Texas 78712, USA*; MICHAEL E. HARDING, *Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76021, Karlsruhe, Germany*; JÜRGEN GAUSS, *Institut für Physikalische Chemie, Universität Mainz, D-55099 Mainz, Germany*.

The Lamb-dip technique was employed to resolve the hyperfine structure of the rotational lines of $D_2{}^{17}O$. The high resolution of such a technique allowed us to obtain the hyperfine parameters (quadrupole coupling of ^{17}O and D, spin-rotation constants as well as ^{17}O-D and D-D direct spin-spin interaction constants) with high accuracy. The experimental determination was strongly supported by highly accurate quantum-chemical calculations of the hyperfine parameters involved. The experimental spin-rotation constants of ^{17}O were used to evaluate the paramagnetic contribution to the magnetic shielding constants, whereas the diamagnetic contribution was accurately determined by means of CCSD(T) calculations. These steps are part of a well-tested procedure, which also involves the determination of vibrational and temperature corrections. The present study is part of a wider project which aims at establishing an alternative experimental absolute NMR scale for oxygen and that has been started with an analogous investigation on $H_2{}^{17}O$.[a]
Due to the lack of information on spectroscopic parameters, the rotational spectrum of $D_2{}^{17}O$ was also investigated at a Doppler-limited resolution, spanning a large frequency range: from the millimeter-wave region up to the THz frequency domain. The recorded transitions allowed to determine rotational and centrifugal-distortion constants to a good accuracy.

[a] C. Puzzarini, G. Cazzoli, M. E. Harding, J. Vázquez and J. Gauss *J. Chem. Phys.* **131**, 234304 (2009).