ABSOLUTE ^{17}O NMR SCALE: A JOINT ROTATIONAL-SPECTROSCOPY AND QUANTUM-CHEMISTRY STUDY

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The Lamb-dip technique has been employed for resolving the hyperfine structure (hfs) of rotational lines of $H_2{}^{17}O$. Hfs is due to ^{17}O for para-$H_2{}^{17}O$ lines and to the ^{17}O and H nuclei for ortho-$H_2{}^{17}O$ lines. The high resolution of such a technique allowed us to obtain the hyperfine parameters to a very good accuracy. The experimental determination has been strongly supported by highly accurate quantum-chemical calculations of the hyperfine parameters involved (spin-rotation constants of ^{17}O as well as H, and ^{17}O-H and H-H direct spin-spin interaction constants). Then, the experimental spin-rotation constants of ^{17}O have been used for evaluating the paramagnetic contributions to the magnetic shielding constants, whereas the diamagnetic ones have been accurately computed 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 overall result is an alternative experimental absolute NMR scale for oxygen.