ROTATIONAL SPECTRUM OF CH_2FI FROM 5 GHZ UP TO 1 THZ: ACCURATE SPECTROSCOPIC AND HYPERFINE PARAMETERS

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Guided by theoretical predictions, the rotational spectrum of fluoroiodomethane, CH_2FI, has been been recorded and assigned. Three different spectrometers have been employed, a Fourier Transform Microwave spectrometer, a Millimeter-/Submillimeter- wave Spectrometer, and a THz spectrometer, thus allowing to record a huge portion of the rotational spectrum, from 5 GHz up to 1 THz, and to accurately determine the ground-state rotational and centrifugal-distortion constants. The hyperfine structure of the rotational spectrum has been investigated by means of the Fourier Transform Microwave spectrometer and the Lamb-dip technique in the millimeter-/submillimeter-wave region, thus allowing the determination of the complete iodine quadrupole-coupling tensor and of the diagonal elements of the iodine spin-rotation tensor. Regarding the quantum-chemical calculations, inclusion of relativistic effects turned out to be essential for obtaining reliable and quantitative predictions for experiment, and they have been accounted for either by means of second-order direct perturbation theory or via a spin-free approach based on the Dirac Coulomb Hamiltonian, both in combination with coupled-cluster techniques to treat electron correlation and sufficiently large basis sets.