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Title:Rotational spectra of rare isotopic species of fluoroiodomethane: Determination of the equilibrium structure from rotational spectroscopy and quantum-chemical calculations
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Abstract:Supported by accurate quantum-chemical calculations, the rotational spectra of the mono- and bi-deuterated species of fluoroiodomethane, CHDFI and CD <inf>2</inf>FI, as well as of the ¹³C-containing species, ¹³CH<inf>2</inf>FI, were recorded for the first time. Three different spectrometers were employed, a Fourier-transform microwave spectrometer, a millimeter/submillimter-wave spectrometer, and a THz spectrometer, thus allowing to record a huge portion of the rotational spectrum, from 5 GHz up to 1.05 THz, and to accurately determine the ground-state rotational and centrifugal-distortion constants. Sub-Doppler measurements allowed to resolve the hyperfine structure of the rotational spectrum and to determine the complete iodine quadrupole-coupling tensor as well as the diagonal elements of the iodine spin-rotation tensor. The present investigation of rare isotopic species of CH<inf>2</inf>FI together with the results previously obtained for the main isotopologue [C. Puzzarini, G. Cazzoli, J. C. Lo´pez, J. L. Alonso, A. Baldacci, A. Baldan, S. Stopkowicz, L. Cheng, and J. Gauss, J. Chem. Phys. 134, 174312 (2011); G. Cazzoli, A. Baldacci, A. Baldan, and C. Puzzarini, Mol. Phys. 109, 2245 (2011)] enabled us to derive a semi-experimental equilibrium structure for

fluoroiodomethane by means of a least-squares fit procedure using the available experimental ground-state rotational constants together with computed vibrational corrections. Problems related to the missing isotopic substitution of fluorine and iodine were overcome thanks to the availability of an accurate theoretical equilibrium geometry (computed at the coupled-cluster singles and doubles level augmented by a perturbative treatment of triple excitations). © 2012 American Institute of Physics.

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