465.
Accession number:13032401
Title:Rotational spectra of rare isotopic species of fluoroiodomethane: determination of the equilibrium structure from rotational spectroscopy and quantum-chemical calculations
Authors:Puzzarini, C. (1); Cazzoli, G. (1); Lo´pez, J.C. (2); Alonso, J.L. (2); Baldacci, A. (3); Baldan, A. (3); Stopkowicz, S. (4); Lan Cheng (4); Gauss, J. (4)
Author affiliation:(1) Dipt. di Chim. G. Ciamician, Univ. di Bologna, Bologna, Italy; (2) Dept. de Quim. Fis. y Quim. Inorg., Univ. de Valladolid, Valladolid, Spain; (3) Dipt. di Sci. Molecolari e Nanosistemi, Univ. Ca Foscari Venezia, Venezia, Italy; (4) Inst. fur Phys. Chem., Univ. Mainz, Mainz, Germany
Source title:Journal of Chemical Physics
Abbreviated source title:J. Chem. Phys. (USA)
Volume:137
Issue:2
Publication date:14 July 2012
Pages:024310 (11 pp.)
Language:English
ISSN:0021-9606
CODEN:JCPSA6
Document type:Journal article (JA)
Publisher:American Institute of Physics
Country of publication:USA
Material Identity Number:DK32-2012-028
Abstract:Supported by accurate quantum-chemical calculations, the rotational spectra of the mono- and bi-deuterated species of fluoroiodomethane, CHDFI and CD_2FI, as well as of the 13C-containing species, 13CH2FI, 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_2FI 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).
Number of references:77
Inspec controlled terms:Doppler effect - Fourier transform spectra - ground states - hyperfine

structure - isomerism - isotope effects - microwave spectra - millimetre wave spectra - organic compounds - quadrupole coupling - quantum chemistry - rotational states - submillimetre wave spectra - terahertz wave spectra - vibrational states
Uncontrolled terms:equilibrium geometry - iodine isotopic substitution - fluorine isotopic substitution - vibrational corrections - least-square fit procedure - isotopologue - iodine spin-rotation tensor - diagonal elements - iodine quadrupole-coupling tensor - hyperfine structure - subDoppler measurements - centrifugal-distortion constant - ground-state rotational constant - terahertz spectrometer - submillimeter-wave spectrometer - Fourier-transform microwave spectrometer - quantum-chemical calculations - rotational spectroscopy - equilibrium structure determination - fluoroiodomethane - rotational spectra - frequency 5 GHz to 1.05 THz
Inspec classification codes:A3310E Rotational analysis (molecular spectra) - A3310G Vibrational analysis (molecular spectra) - A3320B Radiofrequency and microwave molecular spectra - A3325F Nuclear spin interactions, quadrupole effects and nuclear coupling (molecules) - A3520B General molecular conformation and symmetry; stereochemistry - A3520J Molecular barrier heights (internal rotation, inversion); rotational isomerism, conformational dynamics - A3520P Molecular rotation, vibration, and vibration-rotation constants - A3520S Molecular hyperfine and fine-structure constants - A3120 Specific calculations and results for atoms and molecules - A3130G Hyperfine interactions and isotope effects (atoms and molecules) - A3220D Radiofrequency and microwave atomic spectra
Numerical data indexing:frequency 5.0E+09 1.05E+12 Hz
Treatment:Theoretical or Mathematical (THR); Experimental (EXP)
Discipline:Physics (A)
DOI:10.1063/1.4731284
Database:Inspec