FTIR and Raman spectra of CH(D)FCl–CF_2–O–CHF derivatives of enflurane. Experimental and ab initio study.

Autorzy

S. M. Melikova

K. S. Rutkowski

E. Telkova

Bogusława Czarnik-Matusewicz

Maria Rospenk

Wouter A. Herrebout

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Streszczenie

The vibrational spectra of two H/D derivatives of enflurane are studied with the help of FTIR cryospectroscopy in liquefied Kr and Raman spectroscopy of pure liquid. The majority of fundamental bands are identified. Using MP2/6-311++G(df,pd) calculations the six local minima are found on the potential energy surface and ascribed to the most stable conformers of enflurane. The vibrational frequencies, infrared intensities, and Raman activities are found at the same level of theory. The potential energy distribution is calculated for the most stable conformer. Assignment of the vibrational bands registered is performed using the results of calculations of the frequencies with “anharm” option implemented in Gaussian. The model IR and Raman spectra built with the help of data of ab initio calculations reflect the basic features of experimental spectra. IR spectra of cryosolutions of enflurane and acetone in liquefied Kr suggest weak complex formation stabilized by “blue shifting” H bonds.

Słowa kluczowe

Enflurane, IR and Raman spectra, Anharmonicity, Ab initio calculations, Conformation, H bond

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