Towards understanding the spectroscopic features of enflurane. The fundamental and overtone bands of CH stretching vibrations.

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Rok wydania

2014

Czasopismo

Chemical Physics Letters

Numer woluminu

604

Strony

68-71

DOI

10.1016/j.cplett.2014.04.057

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The near-IR and the mid-IR spectrum of enflurane dissolved in liquid Xe was studied at $T \sim 170$ K. Inversion nature of the two CH stretching vibrations were analyzed by comparison of relative intensities of corresponding bands in a range of a first overtone and fundamental transition. The effect was explained by including features of the dipole moment function of enflurane. The analysis of the electro-optic parameters of the stable conformers was done with the help of MP2/6-311++G(df,pd) anharmonic calculations.

Adres publiczny

http://dx.doi.org/10.1016/j.cplett.2014.04.057

Strona internetowa wydawcy

http://www.elsevier.com