HBOND2019

Amsterdam

24-27 SEPTEMBER 2019

Conference Book

23rd International Conference on

"Horizons in Hydrogen Bond Research"

Poster 36

The FTIR spectrum of methoxyflurane and methoxyflurane/dimethyl ether mixtures in cryosolutions. Conformational analysis and evidence of H bonded complex formation

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Methoxyflurane ($CHCl_2CF_2OCH_3$), i.e. 2,2-dichloro-1,1-difluoro-1-methoxyethane according to IUPAC name, is a powerful anesthetic and analgesic agent, presently used as analgesic predominantly. In this report, IR spectra of methoxyflurane and methoxyflurane/dimethyl ether ($(CD_3)_2O$) mixtures are studied with the help of FTIR cryospectroscopy and ab initio calculations. The spectra are measured in liquefied Kr at $T \sim 140 – 160$ K and in liquefied Xe at $T \sim 165 – 195$ K. The most characteristic changes of the IR spectrum are observed in ~3100 ÷ 2800 cm^{-1} region, where stretch CH and CH_3 group vibrations of methoxyflurane are registered. A new band situated at low wave number side of CH stretch is detected in mixtures with $(CD_3)_2O$. Temperature behavior of this band suggests complex formation stabilized by weak H bond. Enthalpy of formation is estimated in series of temperature measurements of the spectra. DFT calculations with wb97xd functional and a set of Pople-type basis sets are performed to find the most stable conformers, geometric and spectroscopic parameters of the systems studied. The most stable heterodimer corresponds to the structure stabilized by C-H…O contact of H-bond-type predominantly. Weaker contacts stabilize additionally the methoxyflurane/dimethyl ether system. The calculated spectroscopic and energetic parameters are in reasonable agreement with those found experimentally.