Vibrational spectra and conformational analysis of desflurane. A cryosolution and ab initio study.

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The vibrational spectra of desflurane are studied with the help of FTIR cryospectroscopy in liquefied Kr at $T \sim 120–160$ K and Raman spectroscopy of pure liquid. Particular IR bands reveal qualitative temperature changes of conformational origin. Only two of the six stable conformers found in MP2/6-311++G(d,p) calculations contribute to the spectra. The calculated vibrational spectra reflect the basic features of experimental spectra. IR spectra of two component cryosolutions suggest weak complex formation between desflurane and methyl fluoride stabilized by ‘blue shifting’ H bonds.

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